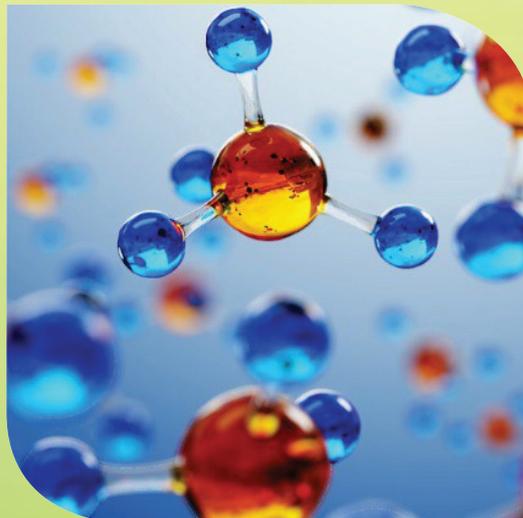
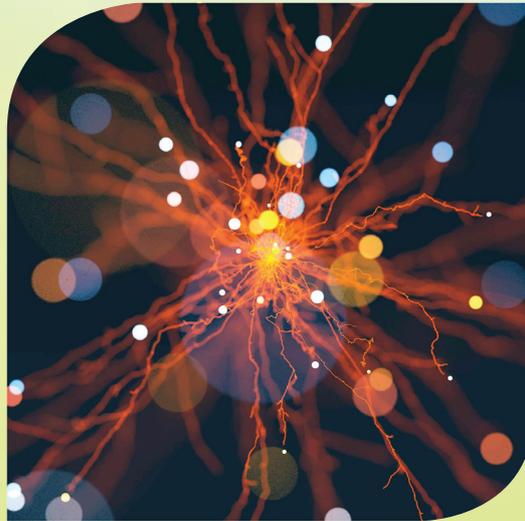


3rd Global Virtual Summit on

CATALYSIS AND CHEMICAL ENGINEERING

**September
12th - 13th, 2022**

BOOK



Theme:

Contemporary
Innovations and
Emerging Novel
Research in Catalysis
and Chemical
Engineering

**CHEMICAL
CATALYST 2022**



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Keynote Forum Day 1

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Dr Zongyou Yin

The Australian National University, Australia

The Roles of Polymorphism in Photo/Electro-Catalysis

The inorganic materials are phase engineerable from crystalline to amorphous solids, i.e. so-called amorphous polymorphism. The polymorphism could play some roles in various applications, e.g. photovoltaics, optoelectronics, and catalysis. In this talk, two kinds of functional condensed/solid materials will be discussed, two-dimensional (2D) semiconductors for photocatalysis and metallic 2D materials for electrocatalysis. Specifically, first, the research on the development of new 2D photocatalysts for photocatalytic methanol storable H₂ fuel production and N₂ fixation will be presented. Our research outcomes indicated the crystalline/amorphous polymorphism and light-responsivity can play the critical roles in designing and developing the efficient photocatalysts. The catalysis stability was also evaluated by extending the working time. Second, transition metal dichalcogenides (TMDs) are known to possess several different (2H, 1T, 1T') phases. To pursue the

highly electrical conductivity and active catalysis, the 1T'-TMDs are especially welcome. However, the synthesis of high-yield single layer TMDs using colloidal strategy is still challenging. This talk will share our recently developed general bottom-up synthesis method under mild conditions to prepare 1T'-TMDs monolayers. Our results showed that the crystalline phase with tensile strain play the critical roles in electrocatalytic hydrogen production.

In short, nanomaterials with rich engineerable parameters, including polymorphism, energy gap, and strain, provide promising avenues to tailor materials functionalities. The explored co-relationships between structuring, reactivity and stability are expected to shed light on the further development of next-generation nanoenergy technologies. This talk highlights the synergistic materials science and engineering can provide the opportunities to customize nanomaterials for advanced modern technology development.

BIOGRAPHY

Dr. Zongyou Yin obtained his B.S. and M.S. degrees at Jilin University in China, and completed his Ph.D. at Nanyang Technological University (NTU) in Singapore. Then, he started his postdoc careers at NTU/Singapore, IMRE/Singapore, followed by MIT and then Harvard University. Dr Yin started his own Research Group at Australian National University (ANU) from 2017. His group's research is interdisciplinary, encompassing AI-driven materials innovations, nano-to-atomic materials science, fundamental relationship among materials-structures-devices, and synergistic integration of multi-functions towards systems for energy and wearable applications. He has been honoured as World Highly Cited Researchers every year since 2015 (Clarivate Analytics).

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Bunsho Ohtani



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Design, Preparation and Characterization of Functional Solid Materials Based on Energy- resolved Distribution of Electron Traps

How can we design functional solid materials, such as catalysts and photocatalysts? What are the decisive structural parameters controlling their activities, performance or properties? What is obtained as structural properties by popular conventional analytical methods, such as X-ray diffraction (XRD) or nitrogen-adsorption measurement, is limited to bulk crystalline structure and specific surface area, i.e., no structural characterization on amorphous phases, if present, and surface structure has been made so far. Recently, we have developed reversed double-beam photoacoustic spectroscopy (RDB-PAS) which enables measure energy-resolved distribution of electron traps (ERDT) for semiconducting materials such as metal oxides [1,2]. Those detected electron traps (ETs) seem to be predominantly located on the surface for almost all the metal oxide particles,

and therefore they reflect macroscopic surface structure, including amorphous phases, in ERDT patterns. Using an ERDT pattern with the data of CB bottom position (CBB), i.e., an ERDT/CBB pattern, it has been shown that metal oxide powders, and the other semiconducting materials such as carbon nitride, can be identified without using the other analytical data such as XRD patterns or specific surface area, and similarity/differentness of a pair of metal-oxide samples can be quantitatively evaluated as degree of coincidence of ERDT/CBB patterns. In this talk, an approach of material design based on the ERDT/CBB-pattern analyses is introduced [3].

[1] Chem. Commun. 2016, 52, 12096-12099. [2] Electrochim. Acta 2018, 264, 83-90. [3] Catal. Today 2019, 321-322, 2-8.

BIOGRAPHY

The research work on material chemistry started in 1981 when he was a Ph. D. course student in Kyoto University. Since then, he has been studying photocatalysis and related topics for 40 years and published more than 300 original papers (h-index: 72). After gaining his Ph. D. degree from Kyoto University in 1985, he became an assistant professor in the university. In 1996, he was promoted to an associate professor in Graduate School of Science, Hokkaido University and was then awarded a full professor position in Institute for Catalysis, Hokkaido University in 1998 and retired at the end of March 2022.

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Catalytic glycerol etherification for oxygenated fuels production

The increase in biodiesel production results in the accumulation of glycerol in large quantities, being the 10 wt% of byproduct of the transesterification reaction for biodiesel production. Although the glycerol has many commercial applications in cosmetic and pharmaceutical industries, the development of new ways of converting it to added values products is necessary to support the eco-sustainability of the global process of biomass transportation. On this account, glycerol etherification represents an important approach to afford compounds that can be used as fuel-additives, intermediates in the pharmaceutical industry, non-ionic surfactants or agrochemicals. Specifically, the transformation of glycerol into oxygenated-fuel additives represents an appealing strategy to gain benefits in terms of environmental compliance and diesel engines efficiency. To date, the catalytic etherification

of glycerol is carried out using isobutylene or tert-butyl alcohol, but recent studies have been addressed towards the exploitation of bio-butanol or bio-ethanol as bio-reactants for a completely biomass-derived product. In presence of alcohols, water is formed as by-product, competing with reactants on the active site adsorption, preventing the total glycerol conversion and the formation of desired poly-substituted ethers. This aspect will be discussed and the use of a batch reactor assisted by a tubular permselective membrane for the removal of water to overcome equilibrium limits and improving poly-ethers productivity will be described. A critical evaluation of the main factors affecting the catalytic reaction will be done with the aim to drive the research towards the design of both an appropriate catalyst and an efficient catalytic process for glycerol etherification.

BIOGRAPHY

Catia Cannilla is researcher at CNR-ITAE since 2008 during her PhD in Chemical Technologies and Innovative Processes. Her scientific interest is addressed in the field of heterogeneous catalysis with reference to the development of catalytic materials (preparation, physico-chemical characterization and testing of powered and structured catalysts) for energetic purposes and preparation of clean alternative fuels: CH₄/H₂ production by supercritical water gasification of waste biomass; MeOH and DME production by CO₂ hydrogenation; biodiesel production by transesterification and esterification reactions; oxygenated additives synthesis by glycerol etherification. She is Scientific Responsible of Research projects and she is Guest Editor of Special Issues for Catalyst and Membrane, Topic Editor for MPDI Journals, Editorial Board Member for Catalyst.

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September 12-13, 2022

Theme: Contemporary Innovations and Emerging Novel
Research in Catalysis and Chemical Engineering

Giorgio Facchetti

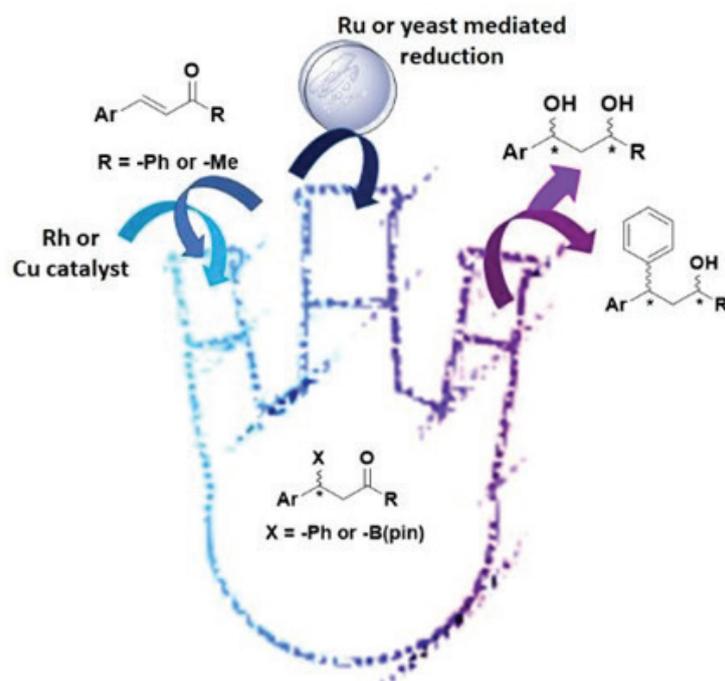
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One-pot reactions in catalysis: a valuable tool for the synthesis of enantiopure intermediates for pharmaceutical applications

One-pot reactions stand out as processes in which several sequential reactions are conducted in a single reaction vessel and most importantly each reaction can only start after the previous one is completed thus leading to the desired final product without the need of any purification of the intermediates. This approach allows in principle to shorten the total synthesis time and generally leads to an increase in the total yield and to a reduction in the amount of chemical waste formed, resulting beneficial from an environmental point of view (*Acc. Chem. Res.* 2021, 54, 6, 1385–1398). Starting from

these concepts of time and pot economy, the combo of chemo- and biocatalytic approach-based on a copper catalyst and *Rhodotorula rubra* yeast respectively- was applied to the stereoselective synthesis of key intermediates such as 1,3 diols in excellent enantio- and diastereomeric excess (*ChemistryOpen* 2018, 7, 393-400). Following the same successful approach, we have recently developed a one-pot reaction in two steps for the preparation of enantio-enriched 3,3-azaaryl-1-aryl-propanols and 3,3-azaaryl-1-alkyl-propanols containing a pyridine core. After the enantioselective addition of the phenylboronic acid to 3-azaarylprop-2-en-1-ones obtained in good yields and enantiopurity by exploiting a chiral

rhodium-diphosphine catalyst (*New J. Chemistry* 2021, 45, 18769-18775), the subsequent carbonyl reduction was carried out by a ruthenium complex for the aryl derivatives or by a *Tourolopsis* genera yeast in the case of the alkyl compounds, thus affording the desired products, key intermediates for pharmaceutical applications.





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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 i.e. artificial metallo-enzymes and metallopeptides, the design and synthesis of new chiral ligands for homogeneous catalysis and with theranostic metal-based complexes.

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Huiyao Wang

Department of Civil Engineering,
New Mexico State University, USA

Photocatalytic membrane reactors for produced water treatment and reuse: Fundamentals, affecting factors, rational design, and evaluation metrics

Treatment and reuse of produced water (PW), the largest wastewater stream generated during oil and gas production, provides a promising option to address the increasing clean water demands. High-performance treatment technologies are needed to efficiently remove the organic and inorganic contaminants in PW for fit-for-purpose applications. Photocatalytic membrane reactor (PMR) is an emerging green technology for removal of organic pollutants, photoreduction of heavy metals, photo-inactivation of bacteria, and resource recovery. This study critically reviewed the mechanisms of photocatalysis and membrane processes in PMR, factors affecting PMR performance, rational design, and

evaluation metrics for PW treatment. Specifically, PW characteristics, photocatalysts properties, membranes applied, and operating conditions are of utmost importance for rational design and reliable operation of PMR. PW pretreatment to remove oil and grease, colloidal and suspended solids is necessary to reduce membrane fouling and ensure optimal PMR performance. The metrics to evaluate PMR performance were developed including light utilization, exergetic efficiency, water recovery, product water improvement, lifetime of the photocatalyst, and costs. This review also presented the research gaps and outlook for future research

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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Dr. Anne M. Gaffney

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Plastic Trash to Monomers and Intermediates – PTMI

To address the issue of waste plastics in landfills, a hybrid approach is proposed. This would use low temperature plasma pretreatment followed by catalytic cracking to augment the conversion of waste polyolefins into monomers, intermediates, new polymers and value-added chemicals. Lightweight packaging (LWP) comprises about 50% of total plastics consumption and consists mainly of single and multilayer films and containers. LWP is heterogenous, contaminated and is difficult to recycle. Mechanical recycling is currently the only commercial approach to recycling but is inadequate to address the growing volume of packaging plastics and degrades or downcycles both polyethylene (PE) and polypropylene (PP). In contrast, feedstock recycling converts polymers to monomer feedstock that can be used to make new products that have virgin-like performance in high volume single use packaging applications, thereby creating new value chains for what is currently a wastestream. Current high TRL feedstock recycling technologies like pyrolysis and gasification are highly energy intensive, require multiple steps (plastics-syngas-methanol-olefins) and have low selectivity to polyolefin building blocks (ethylene, propylene). Alternatively, plastics upcycling aims at selectively deconstructing polymer in a one-step process directly into monomers and high value chemicals (HVC). Consequently, it is proposed

to use a hybrid approach of preconditioning with a low temperature plasma followed by catalytic cracking for conversion of waste polyolefins into monomers, intermediates, new polymers and value-added chemicals. This offers improvement in carbon utilization, cumulative energy demand and selectivity to recycled high value products over current benchmark feedstock recycling processes like gasification and pyrolysis. It is suggested to use LTP treatment as a tunable polyolefin functionalization step to increase selectivity of subsequent catalytic deconstruction and reconstruction. The target waste stream is post-industrial and post-consumer packaging waste, mainly LDPE, LLDPE, and PP films. The primary target products from this novel process are C2-C4 olefins (ethylene, propylene, butylene) which are the raw materials for bulk of the volume of single use plastic production (PE and PP). Aromatic and other HVC precursors like benzene, toluene, xylene (BTX), ethyl benzene and polyols are also expected as by-products from the process. All the products and by-products (C2- C4 olefins, BTX, polyols, HVC) can be upcycled to resins, bulk (polyethylene, polypropylene) and specialty polymers (polyurethanes, epoxy, polyester, Nylon-6) at different market entry points.



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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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Scientific Sessions

Day 1

CHEMICAL CATALYST 2022



Artificial Aging of Crude Oil and Water Remediation by AOPs

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Crude oil in the environment is exposed to a series of weather-climatic factors (water, oxygen, solar irradiation) and microorganisms' action that triggers chemical-physical processes of degradation (known as weathering). In a short time, the original composition of exposed oil can change significantly.

In this work, our research team experimented with an Italian crude oil simulating solar irradiation to understand the modifications induced on its composition by artificial aging. Moreover, we studied the transformations deriving from different advanced oxidation processes (AOP) applied as remediation methods on liquid matrices contaminated by petroleum. For the last objective, we adopted different AOPs (photocatalysis, sonolysis, and sonophotocatalysis). as a photocatalyst, we used TiO₂ immobilized on a non-woven fabric sheet. Crude oil and its water-soluble fractions were analyzed using GC-MS, ¹H-NMR in a liquid state, Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR-MS), and fluorescence. The artificial oil aging induced significant modifications of oil composition with the formation of more oxidized species. All treatments used for the detoxification of polluted water samples, except sonolysis, showed a consistent reduction of organic content with the appearance of potentially toxic substances, confirming that the remediation processes experimented with cannot be applied in natural environments without a careful and repeated experimentation in controlled laboratory conditions.

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 a co-proposer in four national and international research projects, and she coordinated one of them. She is the 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 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).

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The construction of phenanthrene core through a palladium-catalyzed domino approach

Antonia Iazzetti

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One of the most attractive subjects in modern organic chemistry is represented by the development of cascade protocols that, through the sequential multiple bond formation, allow a rapid increase in the molecular complexity of the final products via simple and economic “one-pot” procedures.

Many useful transition metal-catalyzed cascade processes have been developed in this frame with a great part of them based on palladium catalysis. As a sequel to our studies in the construction of polycyclic compounds through transition metal-catalyzed methods, we studied the palladium-catalyzed cascade reaction of deoxybenzoin derivatives to obtain, through a sequence of oxidative coupling/cyclization/oxidation, substituted phenanthrenes. This class of compounds appeared to us very attractive since the phenanthrene core is widely present in several natural products as well as it is resulted highly effective in developing and synthesizing drugs, colorants, plastics, pesticides, and explosives. Through a sequence of experiments aimed at optimizing the reaction conditions as well as at elucidating the reaction mechanism, we developed a new synthetic route affording the privileged scaffold. According to the proposed methodology, several substituted phenanthrene derivatives have been obtained with yields from good to high in the presence of various functional groups including ether, ketone, ester, nitrile, and nitro. The main features of the work will be discussed during the presentation.

Biography

Antonia Iazzetti is professor assistant at the Catholic University of the Sacred Heart of Rome, working in the field of organometallic chemistry. Since her Ph.D. in Pharmaceutical Science at the Sapienza University of Rome in 2013, Antonia Iazzetti focused her research activities on the development of new synthetic methods for the construction of polyfunctionalized molecules of biological interest taking advantage of palladium, copper, and gold catalysis. Recently she has aimed at the valorization of industrial by-products by developing innovative and highly sustainable extraction/purification/concentration technology to be applied to the recovery of valuable compounds from production side-streams. She is involved in international (Horizon 2020) and national (PRIN 2017) relevant research projects that encourage her scientific collaborations with various groups.

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Supported 9-amino-9-deoxy-9-epi-quinine and its co-catalyst on silica: a potential tool in batch and flow heterogeneous reactions

Alessia Ciogli, Andrea Sorato and Martina De Angelis

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Asymmetric organocatalysis is an 'elegant tool' that has allowed chemists to think of new way of putting together molecules. Widely used in research and discovery, organocatalysts result less employed into large scale production yet. The heterogeneous version of organocatalysts gained significant interest in advanced organic chemistry due to its potential in catalyst reuse and easy scale-up (i.e., continuous flow systems). This talk presents the results obtained from the development of organocatalyst based on cinchona alkaloid derivative on silica particles together its acid co-catalyst. In fact, the primary amine requires the presence of an additional acid co-catalyst to well perform. Synthetic protocol was based starting to preparation of mercapto-silica gel followed to the thiol-ene reaction between modified silica and olefinic groups of catalytic system. The solid material has been in depth characterized by elemental analysis, FT-IR and solid-state NMR. The heterogenized catalyst efficiently promoted the reaction of ketones with β -nitrostyrene, with diastereomeric ratio and enantioselectivity comparable to the homogeneous counterpart. Reuse of catalyst and a first application in flow mode were also investigated. As final part, preliminary results of a small library of supported organocatalysts will be presented aiming to obtain a platform to easy evaluate their catalytic performances.

Biography

Assistant Professor in Organic Chemistry, Dep. of Studies and Technologies of Drug, Sapienza University of Rome.

RESEARCH ACTIVITY: The main interests were addressed on i) synthesis of chiral stationary phases for enantiomeric separations, ii) study of molecular recognition processes by HPLC, iii) stereochemical investigation of chiral molecules, specially of stereolabile species through dynamic HPLC and NMR experiments and, more recently, iv) development of supported organocatalysts for asymmetric reactions in heterogeneous systems. These studies are the result of an "interdisciplinary nature" research that affects both the synthetic organic chemistry, the stereochemistry, the chemical of materials and the separation science.

Co-Author of more than 90 publications on international journals. H index = 26 (Scopus font)

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Low quality rapeseed to produce biodiesel-to-diesel fuel mixtures by applying lipase-catalyzed in situ process

Egle Sendzikiene and Migle Santaraite

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It is important that the production of biofuels is sustainable, both from an environmental and energy point of view. Due to poor transport or storage conditions, about 10 % (of the total harvest) of rapeseed loses its quality – the acidity of their oil often exceeds the norms suitable for human or animal consumption. Consequently, these seeds become biological waste, and the right way to reuse them must be found, from an energy and environmental point of view. The use of nonedible oils for biodiesel production would help in solving such problems as high production costs of conventional biodiesel (free or cheap raw material could be used), secondary use of waste, higher economic, energy, environmental and social benefits. Research aim – to analyse the optimal conditions for the lipase-catalyzed simultaneous oil extraction from low quality (high acidity oil) rapeseed and its transesterification (in situ) process by using a mixture of mineral diesel and alcohol (methanol, ethanol or butanol) in order to produce a mineral diesel-biodiesel blend that meets the requirements for biodiesel fuel.

The production of biodiesel was performed by the lipase-catalyzed simultaneous oil extraction and transesterification process in situ with using a mineral diesel (as an extraction solvent), methanol, ethanol or butanol and biocatalyst – lipase. Mineral diesel and rapeseed oil ratio (w/w) of 9:1 was selected for experiments. Eleven biocatalysts – lipases suitable for in-situ processes, were studied. The conversion of rapeseed oil to biodiesel fuel was investigated in the presence of a lipase from Lipozyme TL IM (*Thermomyces lanuginosus*). The optimal conditions (molar ratio of alcohol to oil– 5:1, reaction time 5-7 hours, temperature 25-40 oC, lipase content – 5-6 w%) for the simultaneous oil extraction and transesterification process have been determined. The physical and chemical properties of the produced fuel blends met the requirements of the standards LST EN 14214 and LST EN 590, therefore they can be used in diesel engines.

Biography

Egle Sendzikiene has completed her PhD in Environmental Engineering in 2005. She is the head research fellow and professor at Agriculture Academy of Vytautas Magnus University (Lithuania). She has published more than 50 papers in the scientific journals. E. Sendzikiene has also conducted a number of national and international projects. She has both scientific and practical knowledge of the analysis and usage of renewable energy, biodiesel fuel and biogas.

Migle Santaraite graduated from PhD in environmental engineering field at Agriculture Academy of Vytautas Magnus University in 2021. Her field of study relates to the biodiesel-to-diesel fuel mixtures production by using in situ transesterification process and biocatalysts – lipases. Also, the evaluation of physical and environmental properties of products obtained.

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Development of intrinsic self-healing material for aeronautical applications

Annalisa Mariconda¹, Simona Russo², Elisa Calabrese², Andrea Sorrentino³, Marialuigia Raimondo², Liberata Guadagno² and Pasquale Longo²

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²Salerno University, Italy

³IPCB-CNR, Italy

Self-healing materials have the capacity to restore themselves after damage and/or degradation. They have been developed since the 2000s, and especially an significant expansion in the progress of self-healing composites has been observed for advanced engineering systems.^{1,2} In aeronautical applications, self-healing composite materials have the ability to repair cracks during a flight and extend the lifetime of the components. The general classification of self-healing systems is based on extrinsic or intrinsic healing.³ The intrinsic self-healing involves covalent bonds, weak non-covalent interactions or a combination of both, based on reversible chemistry. Among the reversible interactions, for its dynamic nature, the hydrogen bond is the most well-known and commonly used in the preparation of physical self-healing systems. Our research group is designing and developing a composite material with self-healing ability through H-bonding interactions. The intrinsic self-healing system can heal multiple times through the inherent dynamic network. Preliminary studies were carried out using supramolecular elastomer of polyethylene glycol monomethyl ether methacrylate (PEGMA) and urea-N-2-amino-4-hydroxy-6-methylpyrimidine-N'-(hexametylen-n-carboxyethyl methacrylate) (HEMA-Upy), poly(PEGMA-co-UPy).⁴ The copolymers Poly(PEGMA-co-UPy) were synthesized through three reaction steps with different percentages of HEMA-Upy: 2.5, 5.0 and 7.8 wt %. DMA tests have been employed to assess the auto-repair ability of the samples under dynamic stresses characterized by different frequency values. The copolymer Poly(PEGMA-2.5%-UPy) has been blended with epoxy resins to confer self-healing properties to the resulting composite material, thanks to the reversibility of hydrogen bond interactions.

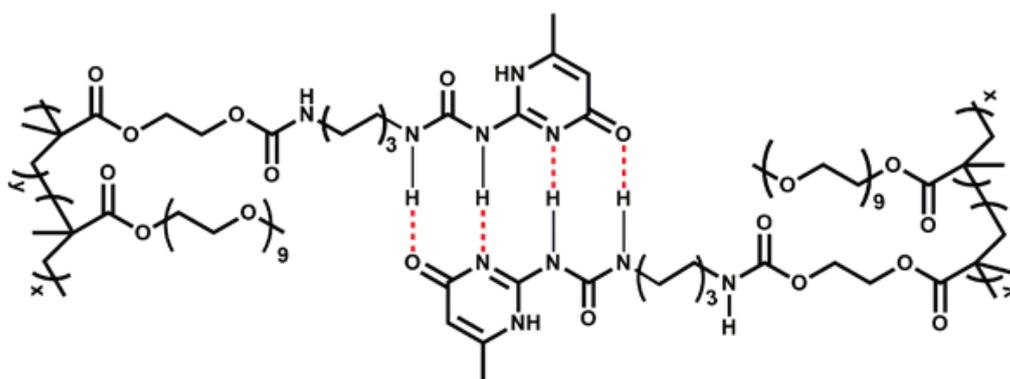


Figure 1. H-bonding interactions between two copolymer chains of Poly(PEGMA-co-UPy).

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Biography

Annalisa Mariconda is associate professor of Inorganic Chemistry at the Basilicata University, Italy. In 2006 she graduated in Chemistry at the Salerno University, Italy. In 2010 she obtained the title of PhD in Chemistry with a thesis on olefin metathesis reactions promoted by new ruthenium-based catalysts. She has been active in the synthesis, characterization and study of new metal complexes in catalysis and their possible use as drugs. From 2012 to 2015 she worked as part of the European IASS (Improving the Aircraft Safety by Self - healing structure and protecting nanofillers) project. Her research activity is documented by scientific papers on international journals as well as by national, European and American patents in collaboration with other research groups.

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Mechanistic Insights on Ethylene Polymerization with Ni(II) Catalysts: the impact of the ligand on the polymer microstructure

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Recently, neutral κ^2 -(N,O)-salicylaldiminato Ni(II) complexes showed to be promising candidates to obtain polyethylene with desired microstructure moving from high-molecular-weight polyethylene to hyperbranched oligomers^(1,2).

Detailed computational studies⁽²⁾ showed that the linear propagation and termination/branches formation mechanisms overlap until the ethylene coordinates with the chain in cis to the oxygen ligand. Then, the reaction proceeds toward the new insertion or a monomer de-coordination. The de-coordination is the key step for a) β -H elimination and 2,1 re-insertion or b) chain transfer reaction. In the de-coordination transition state, the release of the monomer is promoted and made competitive by a weak coordination of the ligand to the metal center, operative only for the case of sufficiently electron-rich ligands

These studies initially performed on 2,6-(3',5'-R₂C₆H₃) substituted systems (Chart A) provided the right insights to extend the discussion to bis(imino)-phenoxy (Chart B) (3) and cyclophane catalysts (Chart C)⁽⁴⁾.

All the results obtained, in agreement with experiments, lead to the same conclusions strengthening our new mechanistic hypothesis and paving the way for the scientific community to exploit this novel concept of design new catalysts tuning opportunely the Ni-ligand interaction on the base of the desired product.

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Biography

Lucia Caporaso on 1996 earned the PhD in Chemistry at the University of Naples with a thesis: "Synthesis of polymers and copolymers of alpha-olefins promoted by Ziegler-Natta metallocene systems" under supervision of Prof. Paolo Corradini. On 1996 she was granted a fellowship from the "Federchimica" and on 1997 from the "Istituto di Chimica Nucleare" of CNR in Rome on the synthesis of deuterate olefines. On January 1998 she won a post-doc fellowship on the topic 'Growth and microstructural analysis of nanosized Y2O3 doped with rare-earths' at the University of Verona. From September 1999 to August 2003 she received a research grant by the University of Salerno. She has been Assistant Professor of Industrial



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Chemistry at Department of Chemistry of Salerno University from 2004 to 2017. Since 2017 she is associate professor at University of Salerno. The main interests of Lucia Caporaso are in the understanding of the mechanics of reactions promoted by transition metals with both computational and experimental approaches.

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Multifunctional Photoelectroactive Platform for CO₂ Reduction

Bahareh Khezri and Lukas Devanosky

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In recent years, CO₂ photo/electroreduction has received great attention due to the urges and concerns to solve problems connected with global warming, for example, reducing the consumption of fossil fuels as energy sources and switching to renewable energy sources. The realization of this technology depends on efficient photo/electrocatalysts with high selectivity for the products. We reported a programmable, bifunctional, scalable, high-performance, and low-cost bioinspired catalyst for photo/electrochemical CO₂ reduction (P/EC-R). We synthesized hydroxyapatite (HAP) needle-like nanoparticles coated with a functional polydopamine polymer (HAP/P(DOPA)) and then modified them with copper nanoparticles (HAP/P(DOPA)/Cu NPs). It was expected that HAP and P(DOPA), due to their plentiful functional groups such as hydroxyl (-OH-), oxygen (-O- and =O), and amines (-NH₂ and -NH-), provide extensive active catalytic sites, participate in the capture, maintenance, and hydrogenation of the CO₂ intermediate, and offer a combination of efficient electrical conduction and photoactivity and synergistic effect together with Cu nanoparticles, thus potentially empowering CO₂ P/EC-R.

Biography

Dr. Bahareh Khezri studied BSc and MSc Chemistry at Isfahan University of Technology and Isfahan University respectively, in Iran. At 2008 she received Singapore International Graduate Award (SINGA) and joined Nanyang Technological University (NTU), Singapore. After PhD graduation she continued as postdoc. In 2015 she joined at the Cambridge Centre for Advanced Research and Education (CARES), in Singapore. In October 2017 she moved to University of the Chemistry and Technology of Prague (VSCHT) as senior scientist. In December 2019 she received a research grant from the Czech Science Foundation (GACR: GACR No. 20-20201S) and continued at VSCHT as Principal Investigator (PI). She will establish her own group at University of Barcelona in September 2022 as RYC researcher. She has published more than 60 research articles in ISI journals.

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Biocatalytic applications: the way forward

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The combination between biocatalysis and continuous processing was identified as one of the foremost key techniques for sustainable manufacturing of fine chemicals. To increase the uptake of biocatalytic processes by industry, it is essential to demonstrate the reliability of enzyme-based methodologies directly applied to the production of high-value products.

The continuous synthesis of different amines and aldehydes was achieved by exploiting the enhanced stability and broad substrate scope of an immobilized transaminase from the halotolerant bacterium *Halomonas elongata*. Various substrates were flow-transformed to the corresponding amines/aldehydes in good-to-excellent-yields, with the reduction of reaction time by 1 to 2 orders of magnitude compared with batch mode.

Subsequently, multi-enzymatic cascade reactions were assembled generating natural metabolites as the powerful antioxidant hydroxytyrosol, hystaminol and triptophol, whose syntheses are completely inefficient due to low yields and long reactions. This strategy mimicking the natural metabolic pathways allowed for their obtainment with excellent yields and residence time at 10 mM scale. This work combined self-sufficient bioreactors (in situ cofactor recycling), with automated systems (in-line work-up and purification), but the most advanced achievement was the *recovery and reutilization of waste waters*, giving rise to ultra-efficient processes.

Finally, multi-gram synthesis of melatonin (so far exclusively chemically produced) and different natural aroma-compounds were performed. The small packed-bed reactor (2 mg of a covalently immobilized acyltransferase from *Mycobacterium smegmatis*) handling high substrate loading (0.5-0.25 M) in 5 min of residence time led to excellent time-space-yield (up to 37 g/day). Again aqueous and organic phases were completely recovered and reuse, giving rise to *virtually zero waste reactions*.

Biography

Martina Letizia Contente is an Assistant Professor at the University of Milan. She graduated in Pharmacy at the same University, where she obtained also her PhD in Medicinal Chemistry. During her years as post doc she had the opportunity to work in different International environments increasing her expertise in the development of intensified and sustainable flow- biobased processes for the preparation of high value molecules. Among her research interests enzyme discovery, protein immobilization and stabilization for continuous processing are the most important.

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Novel promising plasma deposited thin-film nanocatalysts for dry reforming of methane

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The conversion of CH_4 and CO_2 known as the dry reforming of methane (DRM) seems to be an ideal solution for the greenhouse gases utilization as well as the production of syngas that can be used for Fischer-Tropsch synthesis. Although the DRM process is environmentally friendly, it has not been implemented on an industrial level due to problems related mainly to catalyst sintering deactivation and carbon deposition. Therefore, this work is aimed at proposing and developing new plasma deposited thin-film nanocatalysts for DRM reaction.

Plasma-enhanced chemical vapor deposition (PECVD) method has been used to produce tungsten- and cobalt-based thin films on structured support in the form of a wire mesh. Tungsten hexacarbonyl $\text{W}(\text{CO})_6$ and dicarbonylcyclopentadienyl cobalt(I) $\text{CpCo}(\text{CO})_2$ were used as precursors, respectively. By controlling the parameters of deposition, e.g. discharge power, deposition time and flow rate of precursors, different films were produced.

The surface analysis of the films was carried out using X-ray photoelectron spectroscopy (XPS) and scanning electron microscopy (SEM) in terms of their molecular structure and microstructure. The kinetic tests were performed in a tubular reactor at temperatures up to 750°C under atmospheric pressure ($\text{CH}_4/\text{CO}_2 = 1:1$, 25 sccm) using gas chromatography (GC) to analyze the composition of the outlet stream.

The cobalt-based catalyst exhibited high activity at relatively low temperatures (under the experimental conditions, for 500°C : $X_{\text{CO}_2} = 35\%$, $X_{\text{CH}_4} = 32\%$), while the tungsten-based catalyst was slightly less effective in syngas formation. The plasma deposited cobalt- and tungsten-based films are promising nanocatalysts for the DRM process.

Acknowledgments: The study was supported by the Polish National Science Centre, on the bases of the contract no: UMO-2018/29/N/ST8/02403.

Biography

Ryszard Kapica conducts research in the field of chemical engineering with particular emphasis on non-equilibrium plasma engineering, catalysis on materials produced and modified with plasma methods and molecular engineering.

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Keynote Forum Day 2

CHEMICAL CATALYST 2022

Takashi Hisatomi^{1,2}



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²PRESTO-JST, Japan

Particulate Photocatalysts for Renewable Hydrogen Production from Water

Overall water splitting (OWS) using particulate photocatalysts is studied as a means of large-scale renewable solar hydrogen production [1]. Various oxide, (oxy)nitride, and (oxy)chalcogenide semiconductor materials have been studied as photocatalysts. The apparent quantum yield of SrTiO₃ for OWS has been improved to 95% in the near-ultraviolet region by refining the photocatalyst and cocatalyst preparation [2]. Recently, a 100 m² scale solar hydrogen production system consisting of arrayed photocatalytic panels based on modified SrTiO₃ and an oxyhydrogen gas-separation module was built, and its performance was reported [3]. Nevertheless, for practical solar energy harvesting, it is essential to develop photocatalysts that are active under visible light irradiation. Some (oxy)nitride and oxysulfide photocatalysts have been shown to be active in OWS under visible light

irradiation. In addition, two different photocatalysts can be combined so that hydrogen and oxygen are generated on the respective photocatalysts via two-step excitation (also known as Z-scheme). Z-scheme-type particulate photocatalyst sheets consisting of La- and Rh-codoped SrTiO₃ and Mo-doped BiVO₄ split water into hydrogen and oxygen, showing a solar-to-hydrogen energy conversion efficiency exceeding 1.0% [4]. Some other (oxy)chalcogenides and (oxy)nitrides with long absorption edge wavelengths can also be applied to Z-schematic photocatalyst sheets. In my talk, the basics of photocatalytic water splitting and recent advances in photocatalytic materials and reaction systems are presented.

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BIOGRAPHY

Takashi Hisatomi received his PhD in Engineering from the University of Tokyo under Prof. Dr. Domen's supervision in March 2010. He studied as a postdoctoral fellow in Laboratory of Photonics and Interfaces of École Polytechnique Fédérale de Lausanne from April 2010 to March 2012. He moved to the University of Tokyo in April 2012 as a postdoctoral fellow and acquired a position of Assistant Professor in August 2012. He moved to Shinshu University as Associate Professor in April 2018. His major research interests are semiconductor photocatalysts and photoelectrodes for overall water splitting, kinetics and reaction selectivity of photoexcited carriers in semiconductors, and reaction systems and processes for renewable solar fuel production.

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Bismuth oxyhalides as novel adsorptive photocatalysts for water remediation by concentrate and destroy approach

Environmental pollution has become a hot issue in today's world. It is mainly caused by toxic chemicals released in the air, water, and soil, leading to the destruction of biodiversity and the degradation of human health. Pollution levels increase day by day, needing fast and efficient solutions. In the last decades, the scientific community has proposed essential solutions for the depollution of the various matrices employing different approaches. Advanced oxidation processes (AOPs) offer important perspectives in this regard. Photocatalytic degradation has a special place, operating under ambient conditions and degrading many pollutants without the addition of chemical oxidants [1, 2]. However, photocatalytic processes are less effective when used to treat trace concentrations of pollutants in a large volume of contaminated matrices due to: 1) large reactor size (necessity of particular reactor configuration, with consequent increase of the costs),

2) limited light penetration, 3) high energy cost, and 4) difficulties in recycling and reusing the photocatalysts. To facilitate the degradation of traces of pollutants, sophisticated carbon/TiO₂ nanotubes composites have been proposed [3, 4] that combine high adsorption capacity and photoreactivity. In the present study, we report our recent results in the use of BiOX (X = Cl, I, and Br) as novel adsorptive photocatalysts able to concentrate on their surface

different classes of pollutants (polyphenols, drugs, dyes, etc.) also in the dark and degrade them quantitatively after exposure to solar light irradiation.

We thank Velux Stiftung Foundation for the financial support through project 1381 "SUNFLOAT

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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 80 ISI papers, 3 books, 8 book chapters and 2 patents. H-index: 24 (Scopus); 28 (Google Scholar).

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Irmgard Frank

Leibniz University Hannover
Theoretical Chemistry, Germany



Classical description of nuclear motion: Successes and failures

The attempt to explain the chemistry of any kind of matter by a combination of quantum mechanical density functional theory for the electrons and classical Newton dynamics for the nuclei started almost 40 years ago with the work of Car and Parrinello. Since then many molecular systems were investigated. The big success of Car-Parrinello (or ab-initio) molecular dynamics compared to wave packet calculations leads to the thought that there is no reason to describe nuclear motion quantum mechanically. Using a classical approach makes the method deterministic and

free of paradoxa. A lot of phenomena can be explained in this way. However, we are presently not able to explain rotational spectra and low-temperature heat capacities. Further work is necessary to find out if this means a failure of the concept of classical nuclear motion or if our practical many-body calculations are too approximate. In principle, a single confirmed experiment that is not in agreement with the assumption of classical nuclear motion would falsify the complete concept.

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 in the group of Michele Parrinello at the Max-Planck institute in Stuttgart where she developed the restricted-open-shell-Kohn-Sham- Methode (ROKS) for the simulation of photoreactions. In 1998, she went back to Munich and completed her Habilitation in 2004. Her work focused on the simulation of chemical reactions. In 2008 she was appointed associate professor at the University of Hannover.

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Lucia Steenkamp

CSIR, Chemicals Cluster, South Africa



Extraction of ferulic acid using biocatalysis

The environmentally friendly nature of biocatalytic reactions is highly desirable as a green technology with significantly less energy input and waste generation when compared to traditional manufacturing processes.

An optimised process was developed for the extraction of ferulic acid from non-GMO bran. The technology can be broken up into three distinct unit operations, namely: 1] Preparation of the material for extraction, 2] biocatalytic extraction of the ferulic acid and finally 3] downstream processing to purify the product from the reaction mixture.

Milling of the coarse maize bran increased the ferulic acid yield as the finer particles are more accessible to the enzyme for the breakdown of the proteins into smaller units as well as for the

breakage of the ester linkages binding the ferulic acid to the membranes of the cells. The bran is rehydrated with hot water to make access of the enzymes better and rehydration was found to be a crucial step for optimum ferulic acid yield. A single enzyme, Pentopan used in the baking industry at a pH between 6.6 and 7 is used at 60°C. At the end of the reaction with the ferulic acid released, the reaction mixture is filtered and the supernatant added to the Purolite MN150 resin. The ferulic acid is adsorbed onto the resin at 60°C and then the resin is washed with water to remove any other unbound, unwanted products. The ferulic acid is then desorbed with 100% ethanol and treated to remove unwanted sugars and more hydrophilic compounds and recrystallised. HPLC analysis showed more than 95% purity.

BIOGRAPHY

Dr Lucia Steenkamp is a Principal Researcher at CSIR and Director of the Industrial Biocatalysis Hub in South Africa, specialising in Biocatalysis and has been an author and co-author of numerous peer-reviewed papers and two book chapters. She has developed technologies for industry clients in the pharmaceutical, veterinary, biocides, food, flavours and fragrance industries, leading to five granted patents, nine technology demonstrators and five technology packages licensed to external clients. She has won the South African Women in Science Award (SAWISA) for Research and Innovation in 2018 for her work leading to technologies for commercialisation. She has been a finalist in the NSTF rewards in 2012, 2019 and 2020 for the development of new Green technologies.

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Dan Meyerstein

Chemical Sciences Dept., The Radical Research Center and the Schlesinger Family Center for Compact Accelerators, Radiation Sources and Applications, Ariel University, Ariel, Israel, and Chemistry Dept., Ben-Gurion University, Beer-Sheva, Israel.

What are the oxidizing intermediates in the Fenton and Fenton-like reactions?

The Fenton and Fenton like reactions are of major importance due to their role as a source of oxidative stress in all living systems and due to their use in advanced oxidation technologies. For many years, probably till today, there was a debate whether the reaction of $\text{Fe}^{\text{II}}(\text{H}_2\text{O})_6^{2+}$ with H_2O_2 yields OH. radicals or $\text{Fe}^{\text{IV}}=\text{O}_{\text{aq}}$. It is now known that this reaction proceeds via the formation of the intermediate complex $(\text{H}_2\text{O})_5\text{Fe}^{\text{II}}(\text{O}_2\text{H})^+ / (\text{H}_2\text{O})_5\text{Fe}^{\text{II}}(\text{O}_2\text{H}_2)^{2+}$ that decomposes to form OH. radicals or $\text{Fe}^{\text{IV}}=\text{O}_{\text{aq}}$ depending on the pH of the medium. The intermediate complex might also oxidize directly a substrate present in the medium. In the presence of $\text{Fe}^{\text{III}}\text{aq}$ the complex $\text{Fe}^{\text{III}}(\text{OOH})\text{aq}$ is formed.

This complex reacts via $\text{Fe}^{\text{II}}(\text{H}_2\text{O})_6^{2+} + \text{Fe}^{\text{III}}(\text{OOH})\text{aq} \rightarrow \text{Fe}^{\text{IV}}=\text{O}_{\text{aq}} + \text{Fe}^{\text{II}}\text{aq}$. In the presence of ligands often the process observed is $\text{Ln}(\text{H}_2\text{O})_5 - n\text{Fe}^{\text{II}}(\text{O}_2\text{H}) \rightarrow \text{L.} + \text{Fe}^{\text{III}}\text{aq}$. Thus, in the presence of small concentrations of HCO_3^- , i.e. in biological systems and in advanced oxidation processes, the oxidizing radical formed is $\text{CO}_3^{\cdot-}$. Also, the reactions of $\text{Fe}^{\text{II}}(\text{H}_2\text{O})_6^{2+}$ with $\text{HSO}_5^- / \text{S}_2\text{O}_8^{2-}$ in neutral solutions form $\text{Fe}^{\text{IV}}=\text{O}_{\text{aq}}$ or $\text{CO}_3^{\cdot-}$. Clearly in the presence of other transition metal complexes and/or other ligands other radicals might be formed. OH. radicals are clearly often not formed in the Fenton or Fenton like reactions.

Acknowledgement: This study was supported in part by a grant from the Pazy Foundation.

BIOGRAPHY

Born:	Jerusalem, Israel, 1938, Married to Prof. Naomi Meyerstein, 4 children.
1956-61	The Hebrew University of Jerusalem.
1961	M.Sc. in Physical Chemistry (adviser Prof A. Treinin).
1961-65	Soreq Nuclear Research Center.
1963-65	Ph.D. studies at the Hebrew University of Jerusalem (adviser Prof. M. Anbar).
1965	Ph.D. in Chemistry.
1965-6	Research Fellow Argonne National Laboratory, Argonne, IL., USA.
1968-	Chemistry Dept. Ben-Gurion University of the Negev, (1968-83 joint appointment with the Nuclear Research Centre Negev).
1968-73	Senior Lecturer.

- 1973-78 Associate Professor.
- 1978- Professor.
- 1970-71 Coordinator Physical Chemistry Dept. Ben Gurion University of the Negev.
- 1971(summer) N.S.F. Research Fellow at Case Western Reserve University Cleveland, Ohio, USA.
- 1971-74 Consultant Chemistry Division Argonne National Laboratory, Argonne, IL, USA.
- 1973-77 Director Chemistry Dept. Nuclear Research Centre Negev.
- 1976(summer) Visiting Scientist Hahn-Meitner Institut fur Kern Forschung, Berlin, F.R.G.
- 1977-78 Visiting Scientist Argonne National Laboratory, Argonne, IL, USA.
- 1979-89 Library Director, Ben Gurion University of the Negev.
- 1979(summer) Visiting Scientist Argonne National Laboratory, Argonne, IL, USA.
- 1981(summer) Visiting Scientist Argonne National Laboratory, Argonne, IL, USA.
- 1983(summer) Visiting Scientist Argonne National Laboratory, Argonne, IL, USA.
- 1983-95 Full time employment at Ben-Gurion University of the Negev.
- 1983- Consultant Nuclear Research Centre Negev
- 1985(summer) Visiting Scientist Brookhaven National Laboratory, NY, USA.
- 1985- 6 Consultant Netafim, Kibutz Hazerim.
- 1986-91 Chairman Coal Research Center.
- 1987-2010 Irene Evens Professor of Inorganic Chemistry
- 1987(summer) Visiting Scientist Hiroshima University, Japan.
- 1988-91 President, Israel Chemical Society.
- 1990-4 Deputy Rector, Ben-Gurion University of the Negev.
- 1993 Acting President, Israel Chemical Society.
- 1995-2012 President, Ariel University Center of Samaria
- 1997-8 Consultant Makhteshim Ltd.
- 1998-2000 Chairman, Israel Society for Oxygen and Free Radical Research.
- 2000-2002 Secretary Division Inorganic Chemistry, IUPAC
- 2004- Professor Emeritus, Ben-Gurion University of the Negev.
- 2012- Professor of Chemistry, Chemical Sciences Department, Ariel University Member: Israel Chemical Society, American Chemical Society.
- Languages:** Hebrew and English fluent, German good (speaking and reading only).
Over 400 publications, 65 M.Sc. graduates; 62 Ph.D. graduates.
- Honours:**
- 1997 Meitner-Humboldt Research Prize
- 1998 Kolthoff prize
- 2011 Member Academia Europea
- 2017 Israel Chemical Society Prize of Excellence
- 2018 Special issue of J. Coordination Chemistry honoring 80th birthday.
- 2019 Dr. Honoris Causa, Russian Academy of Sciences.
- 2020 Chair Professorship on Hybrid Materials, International and Inter University Centre for Nano-Science and Nanotechnology, Mahatma Gandhi University, Kottayam, Kerala, India.



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Tool to evaluate the personal exposure to atmospheric pollutants. Optimization of the calculation method based on spatial means and surface distributions of the concentrations

Mar Durán, Antonia Baeza and Mercedes Llorens

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Legislation 96/62/EC, 2000/69/EC, RD 102/2011 and RD 39/2017 establish a new strategy for the assessment and management of ambient air quality in Spain. They describe strategies and techniques of measurement to carry out action plans in all the zones that could overpass limit values.

During this study, two-dimensional isoconcentration maps of air concentration values of benzene in the city of Murcia have been elaborated using the Surfer 23.0 program for Windows. This representation provides with an overall vision of the environmental situation, indicates the most affected zones and lets to know the population exposure to air pollutants into the city. Then, a mathematical algorithm Surfer program and mathematical statistical calculations, specifically the areas partial integration method, were used to develop an useful method to calculate the exposure of citizens and benzene average concentrations in each area or district of the city and, finally in the whole of Murcia. This methodology serves to evaluate surface and population distributions of concentrations and to calculate the spatial mean concentration of the area analysed and the average personal exposure. With this work, it has been demonstrated that personal exposure can't be represented by average concentrations in cities, because the distribution of population in the area is not homogeneous.

Finally, from the main results it can be observed the most sensible areas where the exposure of population living there is higher. Also, the whole procedure will provide information for local authorities to take the measures necessary to control sources that contribute to air pollution, such as traffic flow, in order to improve air quality and reduce the citizen exposure.

Biography

Born in Calasparra (Murcia, Spain) on November 11th, 1996. Degree in Chemical Engineering, obtaining the extraordinary end-of-course prize, and Master in Fine and Molecular Chemistry at the University of Murcia. She has received numerous research grants and she is currently contracted as a Phd. Student of Seneca Foundation to carry out her doctoral thesis at the University of Murcia about pollution and environmental management. She is author of high-impact papers: "Advances on kinetics and thermodynamics of non-catalytic supercritical methanol transesterification of some vegetable oils to biodiesel" (Energy Conversion and Management, Elsevier) and "Aggregation of Gold Nanoparticles in Presence of the Thermoresponsive Cationic Diblock Copolymer PNIPAAm48-b-PAMPTMA6" (Polymers, MDPI). She is fluent in Spanish as her mother tongue and has high knowledge in English, Italian and French.

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Liquid phase abatement of formaldehyde with electrospun nanostructured membranes – the synergy of combined AOPs

Carlo Boaretti, Martina Roso, Michele Modesti and Alessandra Lorenzetti

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The present work investigated the effects of the combination of different advanced oxidation processes (AOPs) for the degradation of aqueous solutions with a low concentration (90 ppm) of formaldehyde. To this end several strategies based on the employment of UV photocatalysis, Fenton reaction and ultrasound irradiation were considered along with the use of heterogeneous nanostructured catalysts, supported on polymeric nanofibers. Different heterogeneous catalytic systems based on TiO₂ and FeSO₄ were employed, without the addition of hydrogen peroxide, and tested under UV irradiation by varying the combinations among the various selected AOPs using a batch reactor configuration. The results showed that the combination of AOPs gave a synergy since the presence of iron was beneficial in promoting the photocatalytic activity of TiO₂ while TiO₂ was beneficial in promoting the photo-Fenton reaction. On the other hand, the use of ultrasound significantly increased formaldehyde photocatalytic abatement in absence of FeSO₄, while the employment of sono-photo-Fenton reaction produced a combined synergic effect that reduced the residual amount of formaldehyde to less than 20% after 210 mins. A further analysis showed that only an optimal TiO₂/FeSO₄ ratio on the membrane surface is capable to speed up the process to reach a 99% final conversion for the same reaction time interval.

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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Synthesis of Quinoline based Natural and Unnatural Products Utilizing Palladium Cross-Coupling Chemistry

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A range of natural products, with interesting biological activity, contain the quinoline core structure such as isocryptolepine, neocryptolepine, and cryptolepine. These compounds and their analogues can be prepared from functionalized quinoline starting materials by palladium catalyzed coupling reactions. In this talk focus will be directed towards the preparation of some of these natural products and derivatives thereof and the mechanistic investigations conducted to elucidate their mechanism of formation.

Biography

I am trained in organic synthesis with a PhD from the Research School of Chemistry, Australian National University. After obtaining an independent position my research has mainly focused on four aspects – synthetic organic chemistry, medicinal chemistry, photochemistry, and environmental chemistry. In organic synthesis my research is focused on natural product synthesis with a particular interest for compounds with antimicrobial, anticancer, and antimalarial activity. Palladium cross-coupling reactions are commonly utilized in our synthetic sequences.

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Carbohydrate-based crown ethers

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The most modern, most economical and easiest way to prepare pure enantiomers is the asymmetric synthesis in the presence of chiral auxiliaries or chiral catalysts. Chiral crown ethers are a special type of chiral catalysts that can be used under phase transfer conditions and are capable of inducing asymmetric induction. By asymmetric phase transfer catalysis, chiral epoxides, Michael adducts, cyclopropane derivatives, phosphonates, fluorinated compounds, etc. can be synthesized which are potentially biologically active substances or intermediates. It has been found that the type of the monosaccharide, the substituents on the sugar unit and the side arm on the crown ring, have significant influence on both the yield and the enantioselectivity. It has been proven that the most efficient catalysts are monoaza-15-crown-5 type macrocycles annulated to a monosaccharide unit and incorporating a side arm on the nitrogen with three carbon atom. Therefore, this structural motif was retained and several derivatives of these macrocycles have been synthesized in our research group. A few representatives of the monosaccharide-based crown ethers induced a considerable asymmetric induction in certain reactions (in liquid-liquid and solid-liquid systems). In each asymmetric reaction, different catalysts showed the best results, however, crown compounds incorporating a D-glucose, or a D-galactose moiety proved to be the most efficient catalysts. A $(\text{CH}_2)_3\text{OH}$ substituent on the nitrogen atom resulted in the best enantioselectivity in the liquid-liquid reactions, while in solid-liquid systems, $(\text{CH}_2)_3\text{OCH}_3$ and 2-(3,4-dimethoxyphenyl)ethyl groups also enhanced the asymmetric induction.

Biography

Zsolt Rapi graduated in 2008 from the Budapest University of Technology and Economics as a chemical engineer (MSc). After obtaining his PhD degree in 2012, he continued to work in the research group, first as a research fellow, then as a senior lecturer. He recently became head of the research group. His research topic is carbohydrate-based crown ethers and their application in enantioselective syntheses. He is also involved in teaching of several subjects (lectures, practices and laboratory practices). He is a member of a voluntary organization that provides learning assistance to high school students.

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Influence of Pd electron-density in the hydrodechlorination of chloroform to light olefins

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Catalytic hydrodechlorination (HDC) is a promising technology to treat the dangerous volatile chloroform (TCM) under moderate operating conditions. Light olefins like ethylene and propylene are highly valuable products for the petrochemical industry. In this work, carbon nanotubes (CNT), carbon nanofibers (CNF), and two different Pd precursors (PdCl_2 and $\text{Pd}(\text{NO}_3)_2$) were used for the preparation of the respective catalysts (PdCl/CNT, PdCl/CNF, PdN/CNT and PdN/CNF), which were tested in the HDC of TCM to produce light olefins. The four catalysts were prepared by incipient wetness impregnation with a Pd nominal load of 1 wt. %. The catalysts were characterized by TXRF, XRD, BET, XPS, TEM, TPD N₂, and EXAFS XANES. HDC experiments were performed in a fixed bed micro-reactor using the following conditions: 1 atm, 1000 ppm TCM, 100 N cm³min⁻¹ total flow rate, 300°C, a space-time of 0.2 kg h mol⁻¹, H₂/TCM molar ratios of 10-50. The electron-density of Pd particles followed the order: PdCl/CNT > PdCl/CNF > PdN/CNT > PdN/CNF, inversely to the order of Pd particle size, as found by EXAFS XANES and TEM. The highest electron-density shown by PdCl/CNT, which can be related to a stronger interaction of its smallest Pd particles with the support, favors its highest selectivity to olefins (> 80 %) and contributes to its highest and most stable activity. For the other three catalysts, the formation of PdC_x, which appears as the main cause of catalyst deactivation, was evidenced by EXAFS-XANES and XRD.

Biography

Sichen Liu works as a PhD student in the Department of Chemical Engineering at the Universidad Autónoma de Madrid, doing his predoctoral research project with the reference of PRE2018-084424 (Ministerio de Ciencia e Innovación, Spain). His supervisors are Luisa María Gómez Sainero and María Martín Martínez. He has published 3 scientific articles and done two research stays: the first one at ALBA Synchrotron (Barcelona, Spain) from November 20th to 24th in 2019, to characterize the fresh and used catalyst samples using EXAFS-XANES technology; the second one at the Institut Català d'Investigació Química (Tarragona, Spain) from September 1st to November 30th in 2020 to study the simulation of heterogeneous catalyst systems using the software VASP in the Núria López research group.

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Dehydroisomerisation of α -pinene and limonene to p -cymene catalysed by metal oxides in the gas phase

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ZnO and CdO supported on silica catalysts are demonstrated to be an efficient, noble-metal-free catalysts for one-step dehydroisomerisation of α -pinene and limonene to p -cymene in the gas phase. This is an example of the use of heterogeneous catalysis for the conversion of renewable feedstock into value-added chemicals. The reaction was carried out in a fixed-bed reactor at 370°C to yield 90% of p -cymene at 100% α -pinene conversion over ZnO, and at 250°C to yield 80% p -cymene with CdO at 100% α -pinene conversion. The proposed reaction mechanism involves acid-catalysed α -pinene isomerisation followed by dehydrogenation of p -cymene precursors.

p -Cymene can also be produced by dehydroisomerisation of limonene occurring through double bond migration on acid sites followed by dehydrogenation on metal sites. Limonene dehydroisomerisation reaction was conducted at 300 °C which produced 98% p -cymene with 100% limonene conversion over ZnO and at 225°C to yield 100% p -cymene with CdO at 100% limonene conversion. The catalysts showed stable performance for over 24 hours.

Biography

Aliyah Alsharif is a 2nd year PhD student in the University of Liverpool, UK. She received her MS in 2015 from King Saud University KSU in Saudi Arabia. Then she obtained a scholarship to study for a PhD in the UK. She joined research group of Prof. Ivan Kozhevnikov at the University of Liverpool.

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Copper sulphide nanomaterials as efficient photocatalysts in the treatment of dye polluted wastewater

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The inherent problem associated with the inadequate treatment of industrial wastewater polluted with toxic pollutants is still a cause for concern in most countries. In an attempt to address that issue, two copper(II) complexes, $[\text{Cu}(\text{C}_6\text{H}_8\text{N}_3\text{S}_2)_2]\text{Cl}_2$ (1) and $[\text{Cu}(\text{C}_7\text{H}_{10}\text{N}_3\text{S}_2)_2]\text{Cl}_2 \cdot \text{H}_2\text{O}$ (2), were synthesized from 2-(thiophen-2-ylmethylene)hydrazine-1-carbothioamide (L₁H) and 2-(1-(thiophen-2-yl)ethylidene)hydrazine-1-carbothioamide (L₂H) respectively and characterized using various spectroscopic techniques and elemental analyses. The as-prepared complexes were used as single-source precursors for the synthesis of oleylamine-capped (OLA@Cu_xS_y), hexadecylamine-capped (HDA@Cu_xS_y) and dodecylamine-capped (DDA@Cu_xS_y) copper sulphide nanoparticles (NPs) via the thermolysis method at 190°C and 230°C and then characterized using powder X-ray diffraction (p-XRD), UV-visible spectroscopy, transmission electron microscopy (TEM), and scanning electron microscopy (SEM). The p-XRD diffraction patterns confirmed the formation of crystalline rhombohedral digenite Cu₉S₅ with the space group R-3m. The TEM images showed the formation of nanoparticles of various shapes including hexagonal, rectangular, cubic, truncated-triangular, and irregularly shaped Cu₉S₅ nanomaterials. The UV-visible spectroscopy revealed a general blue shift observed in the absorption band edge of the copper sulphide NPs, as compared to bulk Cu_xS_y, with energy band gaps ranging from 2.52 to 3.00 eV. The nanoparticles obtained at 190°C and 230°C were used as catalysts for the photocatalytic degradation of methylene blue (MB) under UV irradiation. Degradation rates varying from 47.1% to 80.0% were obtained after 90 minutes of exposure time using only 10 mg of the catalyst, indicating that Cu₉S₅ nanoparticles have potential in the degradation of organic pollutants (dyes).

Biography

Mrs Linda Dyorisse NYAMEN is an Associate Professor at the University of Yaoundé I, Cameroon. She obtained her PhD degree in 2013 in Coordination Chemistry/Material Science. She is involved in the synthesis of coordination compounds and their use as single source precursors for the preparation of metal sulphide nanomaterials for potential application as photocatalysts for the degradation of organic pollutants, as antimicrobials and in photovoltaics. Her research group obtained in 2014 the Royal Society- DFID Grant. In 2020, she obtained the OWSD Early Career Women Scientists Grant to develop functionalized nano-photocatalysts for the treatment of industrial wastewater. She is the Vice President of the Cameroon OWSD National Chapter and member of learning societies. She is also involved in mentorship.

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Birth of solids: In situ liquid STEM to reveal the earlier stage of growth of nanocrystals

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Understanding the chemical and the physical processes of nanomaterials (NMs) in liquid media is a crucial challenge and of fundamental interest to modern materials science, chemistry and biology.¹ For example, observing the initial steps of nucleation and the growth of solids and following the exact pathway of the formation of bimetallic NMs are of highest interest. This requires techniques allowing the study of NMs in their liquid environments with the corresponding resolution necessary to observe processes at the atomic scale. Transmission electron microscope (TEM) is a perfect technique with its high spatial resolution, enabling the study of materials at the atomic scale.

In this study, we optimized graphene liquid cell to realize in real time atomic scale observations of nucleation and growth of Pt NPs and the formation of Pt-Pd core-shell NPs in liquid mode. We investigate the exact growth mechanisms of platinum NPs from single atoms to final crystals by in-situ liquid STEM at atomic-scale. After nucleation, we show that the nanocrystals grow via two main stages: atomic attachment in the first stage, followed by the second stage of growth, which is based on particle attachment by different atomic pathways. In addition, we investigated the exact atomic mechanisms underlying the growth of Pt-Pd core-shell NPs, where growth mechanisms of the Pt shell on Pd nanocubes are studied in aqueous solution at the atomic level. We found that Pd-Pt core-shell NPs are formed via two distinct mechanisms: (i) at low concentration of Pt atoms, an ultra-thin skin of only a few atomic layers is formed via atom-by-atom deposition and (ii) at higher concentration of Pt atoms, inhomogeneous islands and thick shells are formed via attachment of Pt clusters.^{3, 4}

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Biography

Dr. Walid Dachraoui is currently a scientist at the Swiss Federal Laboratories for Materials Science and Technology (Empa) in Dübendorf, Switzerland. He received his doctoral degree in physics from the University of Antwerp (2012) at the Electron Microscopy for Materials Science group (EMAT). Dr. Dachraoui's research interests cover various topics in electron microscopy and materials science, such as atomic resolution and low-voltage electron microscopy, as well as in-situ electron



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microscopy. His activity is focused on imaging the growth and degradation of nanomaterials for different applications at the atomic level and imaging battery materials (cathode, anode, and electrolyte) and their interfaces at atomic resolution and in real time during charge/discharge. He has published articles in numerous fields ranging from atomic structure of perovskite-based materials, to in-situ liquid TEM, nanomaterials, in-situ electrochemical TEM, battery materials, and materials for solar cells.

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