

CATALYSISMEET2022

2ND INTERNATIONAL CONFERENCE ON CATALYSIS, CHEMICAL ENGINEERING AND TECHNOLOGY

SEPTEMBER 15-17, 2022 | BARCELONA, SPAIN



ALBEDO MEETINGS

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FOREWORD

It is our pleasure to invite all scientists, academicians, young researchers, business delegates and students from all over the world to attend 2nd International Meet on Catalysis, Chemical Engineering and Technology will be held in Barcelona, Spain during September 15-17, 2022.

CATALYSISMEET2022 Conference provides a platform of international standards where you can discuss and share persuasive key advances in Catalysis, Chemical Engineering and Technology. In addition to Presentations, Workshops, and Discussions, the conference also offers a unique venue for renewing professional relationships, networking and for remaining up-to-date variations in our challenging and expanding discipline.

CATALYSISMEET2022 we have not only increased the number of opportunities for you to network with colleagues from across the world but also introduced more focused sessions that will feature cutting edge presentations, special panel discussions, and livelier interaction with industry leaders and experts.

We're looking forward to an excellent meeting with scientists from different countries around the world and sharing new and exciting results in Catalysis, Chemical Engineering and Technology.

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Plenary Forum

New Perspectives and Insights into Silver Catalyzed Direct Propylene Epoxidation

Dr. Anne M. Gaffney*

University of South Carolina, Columbia, South Carolina, USA

Abstract

A series of Ag-based catalysts were studied for direct PO epoxidation with O₂ as the oxidant. Ag supported on CaCO₃ and α -Al₂O₃ were prepared as base materials to study. Promoters (K⁺, Cs⁺, Mo) and feed additives (EtCl, NO, CO₂) were added to the catalyst and feed stream, respectively, in order to evaluate their effects on PO selectivity and yield. Ball-milling of the catalyst during preparation was a significant factor in ensuring proper blending of promoter species in the Ag particle. Surface characterization (chemisorption, XPS, SEM-EDX), bulk composition characterization (XRD, ICP-OES), and reaction kinetic evaluation were conducted to understand the nature of PO selectivity.

Biography

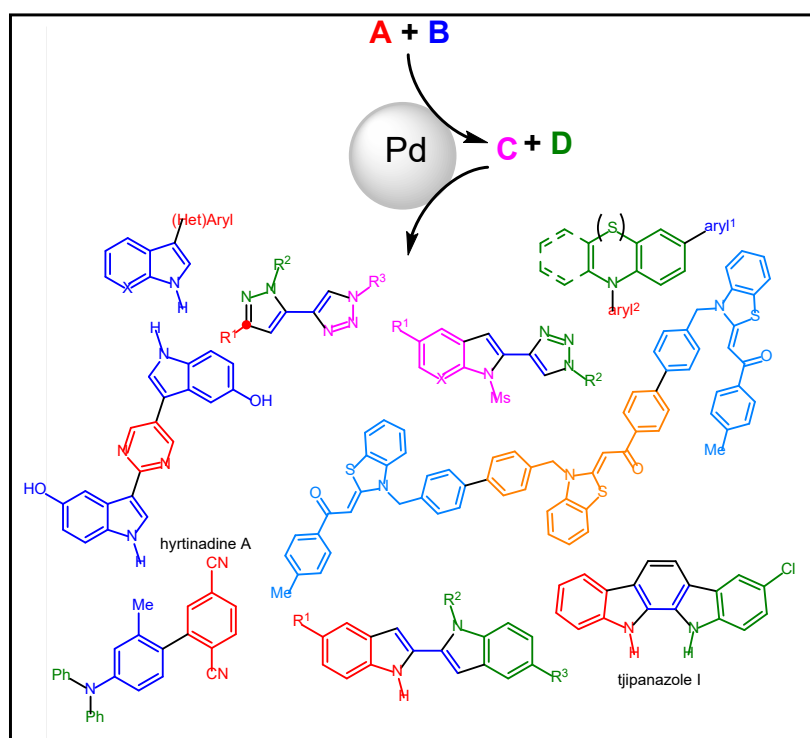
Dr. Anne M. Gaffney is the Chief Science Officer of Idaho National Laboratory and Distinguished National Lab Fellow (2014 – present). She has thirty-four years of experience working in industry inventing and commercializing new technologies for major chemical manufacturing companies including Koch Industries, Lummus Technology, Dow, Dupont and ARCO Chemical Company. She has authored 155 publications and 256 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.

One Catalyst in Multiple Steps in One-pot Fashion- Sequentially Palladium-Catalyzed Processes for the Synthesis of Functional Molecules

Thomas J. J. Müller*

Institut für Organische Chemie und Makromolekulare Chemie, Heinrich-Heine-Universität
Düsseldorf, Universitätsstrasse 1, D-40225 Düsseldorf, Germany

Abstract



One-pot reactions, either in a consecutive, sequential or domino fashion, represent a highly efficient and efficacious synthetic route to many functional molecules in life and materials sciences. Heterocyclic systems cover a vast spectrum of applications and are therefore highly interesting. Recently, transition metal catalyzed multi-component sequences have raised considerable attention since they enable transformations with high tolerance of functional groups. Over the years we have established Pd-catalyzed entries to ynones, diynones, diynes, enals, enones, and boronates, which are valuable intermediates for in situ transformation into complex molecules in a one-pot fashion. Likewise, sequentially Pd-catalyzed processes have opened new avenues to one-pot syntheses of numerous classes of heterocyclic frameworks. Most interestingly, in sequentially Pd-catalyzed processes the same catalyst source acts for a second time without further catalyst addition. This one-pot

methodological concept is most elegantly applied to the syntheses of various classes of functional heterocycles, ranging from functional chromophores to the key steps in very concise syntheses of marine alkaloids, kinase inhibitors and anti-infectiva. By virtue, concise accesses to substance libraries of interest in organic materials and life sciences are efficiently enabled.

Keywords

Cross-Coupling; Heterocycles; Multicomponent Reactions; Sequential Catalysis.

Biography

Thomas J. J. Müller studied chemistry (1984-1989) at the University of München (LMU) (diploma 1989; Ph.D. 1992). After a post-doctoral stay at Stanford University (1993/1994), he developed his independent research at Technical University Darmstadt and LMU (1994-1999; habilitation 2000). After a professorship at the University of Heidelberg (2002-2006) he is a chaired full professor at the University of Düsseldorf since 2006, and since 2019 the spokesman of the Research Training Group 2482 funded by the German Science Foundation (DFG). His research interests encompass synthetic and physical-organic chemistry of functional chromophores, and the design of novel one-pot reactions, documented in more than 300 publications.



Keynote Forum

Absorption from Ultraviolet to Infrared Light for Promotion of CO₂ Reduction with P₄O₁₀/TiO₂

Akira Nishimura*

Division of Mechanical Engineering, Graduate School of Engineering, Mie University, 1577 Kurimamachiya-cho, Tsu, Japan

Abstract

The global average concentration of CO₂ in the atmospheric air has been increasing up to 417 ppmV in December 2021, indicating that it is an increase of 77 ppmV compared to 1980. It is necessary to develop CO₂ reduction technologies to prevent the continues rise of global temperature. Many researches have investigated that CO₂ can be converted/reduced into fuel species such as CO, CH₄, CH₃OH, and so on, by photocatalyst. TiO₂ is one of popular photocatalysts applied for CO₂ reduction. Pure TiO₂ can work under ultra violet (UV) light illumination condition only. UV light accounts for 4 % only in sunlight. If we could use the visible (VIS) light and infrared light (IR) which accounts for 44 % and 52 % of solar energy reaching the earth for photocatalytic CO₂ reduction, it would promote the photocatalytic CO₂ reduction performance significantly. Additionally, it can be claimed that the whole solar energy can be utilized for the photocatalytic CO₂ reduction.

As to the photocatalytic studies on extending the absorption of light wavelength from UV to VIS, many approaches have been tried. One of the popular attempts is a metal doping. Cu, Fe, Pd, Pt and etc. are used as a dopant. As to the photocatalytic studies on extending the absorbed wavelength up to IR, there are some reports. W₁₈O₄₉/g-C₃N₄ composite, WS₂/Bi₂S₃ nanotube and CuInZnS decorated g-C₃N₄ have been reported.

Though several studies on extending the absorbed light of wavelength up to IR have been reported, there is no report investigating the extension of light absorption performance of TiO₂ up to IR. Therefore, this study attempts to extend the light absorption performance of TiO₂ up to IR. P has a layer structure absorbing the light whose wavelength is from UV to IR. Therefore, this study investigates the preparation procedure of P/TiO₂ and its CO₂ reduction performance under IR light illumination condition.

The purpose of this study is to investigate the CO₂ reduction performance of P/TiO₂ changing the wavelength of illuminated light by UV+VIS+IR, VIS+IR and IR only. This study also investigates the impact of molar ratio of CO₂/H₂O or CO₂/NH₃ on the CO₂ reduction characteristics of P/TiO₂. For the photocatalytic CO₂ reduction reaction, a reductant is important since it is a partner for CO₂.

As a result, it is confirmed that the CO₂ reduction with P₄O₁₀/TiO₂ film could occur under the illumination condition of not only UV + VIS + IR but also VIS + IR and IR. Regarding the ratio of CO₂/H₂O, the largest CO₂ reduction performance is obtained at CO₂ : H₂O = 1 : 1 irrespective of light illumination condition, which is the same as the theoretical molar ratio to produce CO. Regarding the ratio of CO₂/NH₃, the largest

CO₂ reduction performance is obtained at CO₂ : NH₃ = 3 : 2 irrespective of light illumination condition, which is the same as the theoretical molar ratio to produce CO.

Keywords

P4O₁₀/TiO₂ Photocatalyst; CO₂ Reduction; Visible Light; Infrared Light

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 88 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.

Enzyme-Sulphide Coupling for Light-Induced Water Splitting and CO₂ Reduction

R. Lucena¹, C. Tapia¹, C. Jarne¹, L. Paul¹, M. Osgouei¹, S. Zacarias²,
I.A.C. Pereira², S. Shleev³, **J.C. Conesa**^{1*}, M. Faraldos¹, M. Pita¹, A.L.
De Lacey¹

Instituto de Catálisis y Petroleoquímica, CSIC. Madrid, Spain¹

ITQB, Universidade Nova de Lisboa. Oeiras, Portugal²

Biomedical Science, Faculty of Health and Society, Malmö University, Malmö. Sweden³

Abstract

Many sulphide semiconductors are photocatalytically active in significant ranges of the visible spectrum; our group has shown this, specifically, for In₂S₃ and SnS₂ (R. Lucena et al., Catal. Commun. 2012, 20, 1; *ibid.* Appl. Catal. A: General, 2012, 415-416, 111). Furthermore, by including V in these sulphides we have shown how their photocatalytic activities can be further extended to even the NIR range (P. Wahnón et al., Phys. Chem. Chem. Phys. 2011, 13, 20401; R. Lucena et al., J. Mater. Chem. A 2014, 2, 8236). Here we will show how coupling these sulphides with enzymes of hydrogenase or laccase types allow photo evolving H₂ or O₂.

First, we could show that combining In₂S₃ with a hydrogenase it was possible to generate photocatalytically H₂ in presence of a sacrificial agent (C. Tapia et al., ACS Catalysis 2016, 6, 5691). Then, we showed that combining In₂S₃ with a laccase it was possible to generate O₂ photoelectrochemically (C. Tapia et al., ACS Catalysis 2017, 17, 4881), this being the first time that such enzyme-sulphide combination allowed photoevolution of O₂. A similar photoelectrochemical generation of O₂ could be shown by combining SnS₂ with a laccase enzyme (C. Jarne et al., ChemElectroChem 2019, 9, 2755).

Some of us carried out recently work which coupled an electrode with a formate dehydrogenase enzyme, including W as active species, so that it was possible to reduce electrocatalytically CO₂ to formate (J. Álvarez-Malmagro et al., ACS Appl. Mater. Interfaces 2021, 13, 11891). Ongoing work will be shown here in which combining this latter enzyme with In₂S₃ nanoparticles allows to perform the same task photocatalytically.

Synthesis of Sulfurated Heterocycles by Pd-Catalyzed Carbonylation under Aerobic Conditions

Raffaella Mancuso*

Laboratory of Industrial and Synthetic Organic Chemistry (LISOC)-Department of Chemistry and Chemical Technologies, University of Calabria, Arcavacata di Rende (CS), Italy

Abstract

The PdI₂/KI-catalyzed oxidative carbonylation of alkyne derivatives suitably substituted with a nucleophilic group -YH (Y = O, NR) has proved to be a powerful methodology for the construction of functionalized heterocycles in a multicomponent fashion starting from simple building blocks. Oxidative carbonylations are carried out in the presence of an external oxidant, necessary to reoxidize the Pd (0) formed in the course of carbonylation to catalytically active Pd (II). This kind of reactivity, unfortunately, cannot be applied to substrates bearing a thiol nucleophilic group (Y = S), owing to the well-known instability of the -SH group to oxidizing agents, including oxygen. This problem has so far hindered the development of PdI₂/KI-catalyzed oxidative carbonylation processes for the synthesis of sulfurated heterocycles. In this Keynote it will be shown the synthesis of different types of molecules, containing sulphur, by Pd-catalyzed oxidative carbonylative process, starting from suitable acetylenic substrates bearing a masked thiol function, still nucleophilic enough to promote a carbonylative S-cyclization process, but sufficiently stable under the oxidative conditions.

Biography

Prof. Mancuso received the PhD in “Methodologies for the Development of Molecules of Pharmacological Interest” at the University of Calabria (2006). She won a “young investigator research project” for the “Synthesis of heterocyclic derivatives of pharmacological interest by metal-catalyzed heterocyclization-carbonylation reactions” (2007). After a post-doc stage at Iowa State University (USA) with Prof. Richard Larock (2008) working in novel iodocyclization reactions, she came back to University of Calabria working on organic synthesis. She joined the group of Prof. Daniel Solé (University of Barcelona-Spain) working on novel syntheses of heterocycles (2012). In 2018 she received her second PhD degree in “Environmental, Construction and Energy Sciences and Engineering” at the University of Calabria. She is currently Associate Professor at the University of Calabria (Italy). Prof. Mancuso received a “Research Award” in September 2017 from the Italian National Consortium in the field “Innovation in Organic Synthesis”. Prof. Mancuso current scientific production include 122 papers in international peer-reviewed journals, 8 patents and more than 170 communications in national or international conferences. She is an international referee in the field of Multidisciplinary and Organic Chemistry, an editorial board member of reputed international journals and Country Editor of an international journal. Her current research interests include organometallic catalysis for the synthesis of high value molecules of pharmacological interest, use of nonconventional solvents in advanced organic synthesis and synthesis of novel materials for advanced applications and for cultural heritage.

Oxidative Dehydrogenation of Cyclohexene on Atomically Precise Subnanometer Cu, Pd and Cupdclusters: Controlling Catalyst's Performance by Cluster Size, Atomic Composition and Support

Stanislav Valtera¹, Juraj Jašík¹, Mykhailo Vaidulych¹, Joanna Elżbieta Olszówka¹, Muntaseer Bunian², Yu Lei², Avik Halder³, Hana Tarabková⁴, Magda Zlámalová⁴, Martin Jindra^{4,5}, Ladislav Kavan⁴, Otakar Frank⁴, Stephan Bartling⁶, Štefan Vajda^{1*}

¹Department of Nanocatalysis, J. Heyrovský Institute of Physical Chemistry v.v.i., Czech Academy of Sciences, Dolejškova 2155/3, 182 23 Prague 8, Czech Republic

²Department of Chemical and Materials Engineering, The University of Alabama in Huntsville, Huntsville, Alabama 35899, United States of America

³Materials Science Division, Argonne National Laboratory, 9600 South Cass Avenue, Lemont, Illinois 60439, United States of America

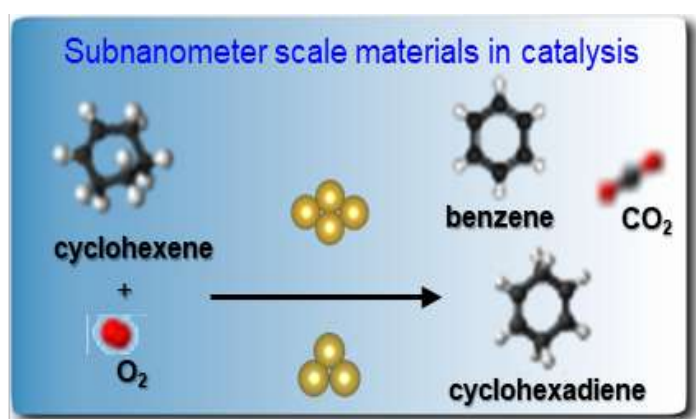
⁴Department of Electrochemical Materials, J. Heyrovský Institute of Physical Chemistry v.v.i., Czech Academy of Sciences, Dolejškova 2155/3, 182 23 Prague 8, Czech Republic

⁵Department of Physical Chemistry, University of Chemistry and Technology in Prague, Technická 5, 166 28 Prague, Czech Republic

⁶Leibniz Institute for Catalysis (LIKAT), Albert-Einstein-Strasse 29a, D-18059 Rostock, Germany

Abstract

A use of a combination of control knobs for fine-tuning of the activity and selectivity of subnanometer clusters in the structure-sensitive reaction of cyclohexene dehydrogenation will be demonstrated by



Scheme 1. Oxidative dehydrogenation of cyclohexene.

(1) the effect of cluster size and support on activity in benzene formation on the example of 1 to 7 atom copper clusters[1] and 1-, 2- and 4- atom Pd species [2] and (2) the effect of cluster composition and of the support on the catalytic activity of mixed 4-atom Cu_{4-n}Pd_n (1 ≤ n ≤ 3) clusters, allowing for a switch in selectivity from benzene to cyclohexadiene with precise changed Pd:Cu atomic ratio in the cluster. [2]

References

[1] “Atom by Atom Built Subnanometer Copper Cluster Catalyst for the Highly Selective Oxidative Dehydrogenation of Cyclohexene”, S. Valtera, J. Jašík, M. Vaidulych, J. E. Olszówka, M. Zlámalová, H. Tarábková, L. Kavan, and Š. Vajda, *J. Chem. Phys.* 156, 114302 (2022), DOI: 10.1063/5.0065350

[2] “Oxidative dehydrogenation of cyclohexene on atomically precise subnanometer Cu_{4-n}Pd_n(0 ≤ n ≤ 4) tetramer clusters: The effect of cluster composition and support on performance”, J. Jašík, S. Valtera, M. Vaidulych, M. Bunian, Y. Lei, A. Halder, H. Tarábková, M. Jindra, L. Kavan, O. Frank, S. Bartling, Š. Vajda, *Faraday Discuss.*, in press.

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Invited Forum

Transparent, Immobilised Photocatalysts for Pollutant Degradation Based on Modified Titania Nanostructured Thin Films

Andreja Gajović^{1,*}, Tihana Čižmar¹, Tayebah Sharifi¹, Vedran Kojić¹, Mario Bohač¹, Krešimir Salamon¹, Krunoslav Juraić¹, Lucija Radetić², Jan Marčec², Ivana Grčić²

¹Ruđer Bošković Institute, Bijenička cesta 54, Zagreb, Croatia

²University of Zagreb, Faculty of Geotechnical Engineering, Hallerova aleja 7, Varaždin, Croatia

Abstract

Nanostructured TiO₂ has taken the scientific focus because of the large specific surface area compared to bulk, increased photo-induced reactions, light absorption, photo-generated charge carrier densities, photo-reduction and contact with pollutants in photo-catalysis. TiO₂ nanostructures, in general, have drawbacks in photo-catalysis, since their wide band gaps (anatase $E_g = 3.2$ eV, rutile $E_g = 3.0$ eV) limit absorbance of the complete solar spectrum and lead to fast recombination of photo-generated electron–hole pairs. Properties of nanostructured TiO₂ materials can be improved by doping or decorating with other materials.

In this study, the photocatalytic degradation of water and air pollutants was examined using transparent immobilized thin films of TiO₂-based nanostructures altered by different modifiers (tungsten, barium and copper-based compounds). An immobilized photocatalysts were designed for the flow-through reactor using simple, inexpensive and fast synthesis. The strategies used for the improvement of their photocatalytic activity will be presented.

A series of transparent porous thin films ($W_xTi_{1-x}O_2$) were obtained by co-sputtering tungsten-titanium in different atomic ratios on FTO glass and then anodizing them in ethylene glycol solution containing NH₄F. The transparent TiO₂ nanotubes arrays (TNT) modified with Cu-based compound were obtained in 2 steps: (1) anodization of the titanium layer on FTO glass prepared using radio frequency magnetron sputtering and (2) modification with different concentrations of Cu(NO₃)₂·3H₂O by wet-impregnation method. For Ba-modified TNT, after the same first step, modification was obtained by annealing solutions of Ba(OH)₂ in different concentrations spin coated on TNT. The morphology and structure of thin films were characterized by SEM, XRD and Raman spectroscopy. Different techniques were used for optical and photo-electrochemical characterization. The photocatalytic activity of $W_xTi_{1-x}O_2$ under solar irradiation was studied using methylene blue as the target pollutant. Ba-modified TNT was studied for degradation of diclofenac in water, while Cu-modified TNT had dual use; degradation of NH₃ and relative humidity sensing.

The photocatalytic activity of TiO₂-based nanostructures was considerably increased by doping or surface modifications. Thus, W_xTi_{1-x}O₂ porous thin film with 1% W showed the maximum photocurrent, while photoelectrochemical results revealed that the charge recombination decreased with increasing the amount of W. MB degradation using W_xTi_{1-x}O₂ was performed at different pH and an enhanced photodegradation rate was obtained at higher pH. Among Ba-modified TNT the most efficient photocatalyst was the sample prepared with 25 mM Ba(OH)₂ which showed 90% diclofenac degradation after 60 min. This result was in agreement with cyclic voltammetry that showed the largest increase in photo-oxidation current densities for the same sample due to the increased photogeneration of ·OH radicals and efficient charge separation. The TNT modified with 2M of Cu(NO₃)₂·3H₂O demonstrated improved ammonia oxidation and superior relative humidity sensing properties. That is a consequence of successful charge carrier separation, which increased the ·OH radicals generation responsible for NH₃ oxidation. The same sample showed the most pronounced increase in the humidity that is related to increase in the concentration of charge carriers on the surface of the sample. The mechanism behind the improvement in photocatalytic activity will be discussed in the view of morphology and structure.

Keywords

Photocatalytic Pollutant Degradation; Transparent TiO₂ Nanotubes Arrays; Tungsten Doping; Barium And Copper Modification.

Funding:

This work was supported by the Croatian Science Foundation under the project HrZZ-IP-2018-01-5246 and by European Regional Development, Fund (ERDF) under the projects “Waste & Sun for photocatalytic degradation of micropollutants in water” (OS-Mi), KK.01.1.1.04.0006.

Biography

Andreja Gajović, senior scientist and Head of the Laboratory for Energy Conversion Materials and Sensors, Division of Materials Physics, at Ruđer Bošković Institute, was obtained her PhD in physics at 2003 at University of Zagreb, Faculty of science. She spent one year at Institute Jožef Stefan in Ljubljana where she specialized in Transmission electron microscopy techniques. Her main field of research is study of nanostructured metal oxides for photocatalytic, photovoltaics and sensors. She published more than 100 papers in peer-reviewed journals and led more than 20 projects.

Monomeric (VO₂⁺) and Dimeric Mixed Valence (V₂O₃³⁺) Vanadium Species at the Surface of Shape Controlled TiO₂ Anatase Nano Crystals

Anna Maria Ferrari*, Eleonora Romeo, Valeria Lagostina, Valter Maurino, Mario Chiesa

Department of Chemistry, University of Torino, via P. Giuria 5, 10125, Torino, Italy

Abstract

Metal atoms and ions at well-defined anatase TiO₂ crystals with exposed (101) and (001) facets represent a promising platform for fundamental studies in catalysis using model systems of high complexity for the development of novel catalytic systems exhibiting higher than usual activities. Herein, we report the geometric and electronic structures of supported paramagnetic vanadium catalysts obtained by reaction of VCl₄ vapors with shape controlled anatase TiO₂ supports with preferential (101) and (001) facets. Electron Paramagnetic Resonance (EPR) spectroscopy and Density Functional theory (DFT) calculations reveal the presence specific monomeric (VO₂⁺) and dimeric mixed valence (V₂O₃³⁺) species with molecular structures dependent on the TiO₂ surface termination.

Keywords

DFT Calculations; Catalysis; Vanadyl; Tio₂

Biography

Anna Maria Ferrari is associated professor at the Chemistry Department of the University of Torino. She works on DFT simulations of materials, surface and interfaces, adsorption and catalysis. Some recent publications:

Monomeric (VO₂⁺) and dimeric mixed valence (V₂O₃³⁺) vanadium species at the surface of shapecontrolledTiO₂ anatasenano crystals *JournalofCatalysis* 2022 10.1016/j.jcat.2021.12.029

Effect of Internal Donors on Raman and IR Spectroscopic Fingerprints of MgCl₂/TiCl₄ Nanoclusters Determined by Machine Learning and DFT *Materials* 10.3390/ma15030909

The NV—...N⁺ charged pair in diamond: a quantum-mechanical investigation *Physical Chemistry Chemical Physics* 2021 10.1039/D1CP02363B

Catalytic Assisted Non Thermal Plasma Process for Removal of Organic Pollutants from Water

G. Iervolino^{*1}, V. Vaiano¹, V. Palma¹

¹Department of Industrial Engineering, University of Salerno, Via Giovanni Paolo II, 132, 84084 Fisciano (SA), Italy.

Abstract

Pollution damages our health and the environment around us. It is the leading environmental cause of numerous mental and physical illnesses and premature deaths, particularly among children, the elderly and people with certain diseases. In addition to affecting human health; pollution is a major cause of biodiversity loss. It reduces the ability of ecosystems to perform useful functions such as carbon sequestration and decontamination.

In recent decades, attention has grown a lot towards chemical pollution of surface, coastal and marine waters underground. A phenomenon that represents a threat to the aquatic environment and that involves effects such as acute and chronic toxicity in aquatic organisms is the accumulation of pollutants in ecosystems and the loss of habitat and biodiversity. Of concern are the effects on human health that can derive from the prolonged presence in aquatic environments of multiple substances. The contamination of water caused by heavy metals, industrial chemicals (including dyes), drugs for human and animal use, herbicides, insecticides up to body care or sun creams therefore represent an environmental problem “Emerging”. Various physico-chemical techniques like adsorption, membranes, and advanced oxidation processes (AOPs) like photocatalysis, UV / ozone, ultrasonication have been tested for the removal of water bound pollutants.

Among these, the non-thermal plasma is very promising and interesting. It is an ionized gas generated by a high voltage electric discharge, capable of generating highly reactive oxidative species (eg OH •, O, HO2 •, H2O2, O2⁻, etc.) and reductive species (eg free electrons, aqueous electrons eaq, H, etc.). Both play an important role in the degradation of reactive and oxidizing organic compounds in water.

Even if very effective, this process has some advantages which are not negligible, in particular the high energy consumption and the probable presence of the reaction by-products. To try to overcome these drawbacks, there are several proposals in the literature to combine NTP with a catalyst. The use of a heterogeneous catalyst can be foreseen both inside the reactor where the electric discharge takes place, and outside the reactor. The presence of a catalyst promotes the

formation of reactive species, increases the half-life and allows better results to be obtained, in less time and by exploiting lower energy values.

The objective of this work is to make a comparison between the catalytic active species most proposed by the literature to improve the performance of NTP for water treatment, to evaluate its efficiency in terms of any developed by-products and required energy consumption. Furthermore, the authors want to examine the recyclability of the proposed catalysts and identify a combination of process parameters that allow to develop an effective treatment for different classes of organic substances dangerous for the aquatic environment.

Biography

Giuseppina Iervolino was born in 1987 and graduates at “University of Salerno” with honors in Environmental Engineering in 2013, with the thesis entitled “Removal of arsenic from drinking water by a photocatalytic oxidation and adsorption process”. In 2017, at University of Salerno, she obtained the PhD title in “Industrial Engineering” (Chemical Engineering curriculum) with the thesis entitled “Advanced Oxidation Processes for Food Industry Wastewater Valorization and Treatment “. From 2017 at July 2019 she was Research Fellow at University of Salerno and actually she is “Assistant Professor” at the Department of Industrial Engineering of the University of Salerno. In 2018 she won the award for best PhD thesis on advanced oxidation processes conferred by the “International PhD School on the Advanced Oxidation Processes”. Her research activity is focused on environmental issues concerning the water treatments (both wastewater, both for drinking purposes) and the valorization, with H₂ production, of organic substances present in the industrial wastewater, with particular reference to the application of advanced oxidation processes, studying innovative catalysts and photocatalysts, the reactor configurations and light source. In addition, she is working on two innovative research line: the application of “Non Thermal Plasma” technology for the removal of not easily biodegradable contaminants (dyes and emerging contaminants) from wastewater, and the electrification of industrial processes for hydrogen production. The results achieved in the context of scientific activity carried out by Dr. Giuseppina Iervolino were published in international scientific journals. Dr. Giuseppina Iervolino participated, presenting communications, at various conferenc. Giuseppina Iervolino is the author, at the month of December 2021, of 44 publications with indexing SciVerse Scopus®, with ISBN / ISSN and DOI number with 992 citations and h-index of 18.

Neoteric Solvents are a Promising Framework for Biocatalytic Processes

María S. Álvarez^{1,2*}, Francisco J. Deive^{1,2}, María A. Longo^{1,2}, Ana Rodríguez¹

¹Department of Chemical Engineering, Campus As Lagoas-Marcosende, 36310 Vigo, España.
²CINTECX, University of Vigo, Campus As Lagoas-Marcosende, 36310 Vigo, España.

Abstract

In recent times, biocatalysis has played a fundamental role in the design of sustainable processes for obtaining molecules of industrial interest or reactions as an alternative to chemical catalysis. Enzymes are considered in the chemical industry as environmentally friendly and clean biocatalysts. However, their varying stability in catalytic reactions, high cost of production and low product yield are often considered a limitation. Despite these weaknesses, biocatalysts are considered potential alternatives to their chemical analogues and much effort is still demanded to improve the performances of biocatalytic processes in several applications like biodiesel production, wherein immobilized and recyclable biocatalysts are imperative [1]. To improve enzyme performance and exploit the potential application at industrial scale, attempts have been put forward on improving the molecular interaction between enzymes and solvents [2]. In the light of these considerations, neoteric solvents as ionic liquids (ILs) and deep eutectic solvents (DESs) appear to be promising candidates to preserve enzymatic activity, as well as an attractive alternative to offset the ungreenness and environmental impact of conventional organic solvents [3]. These neoteric compounds may play different roles in biocatalytic reactions such as solvents or co-solvents. Industrial biotechnology is the main way to obtain biocatalysts, although the upstream and downstream stages in biotechnological processes depict challenges for designing more competitive processes due to the multiple stages required to obtain pure biomolecules. Although there are many alternatives for biocatalysts separation from culture broths, aqueous biphasic systems (ABSs) are considered a feasible method for enzymes extraction in downstream stages due to a number of advantages like the existence of an aqueous environment more biocompatible with enzymes, the possibility of tailor-designing the immiscibility region by an appropriate combination of phase forming compounds or low energy requirements.

In this lecture, we will present and discuss the results obtained from our research where we demonstrate the feasibility of using ILs and DESs as salting-out agents in extraction strategies [4, 5] and co-solvents for biocatalytic reactions like biodiesel production, allowing a step ahead towards a proposal to design one-pot one-step biotechnological processes [6].

Keywords

Biocatalysis; Lipases; Neoteric Solvents; Aqueous Biphasic Systems.

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Ozone and Novel plasma-Deposited Catalysts Applied for Micro pollutants Degradation: Synergy Effect

Marta Gmurek^{1*}

¹Faculty of Process and Environmental Engineering, Department of Molecular Engineering
Lodz University of Technology, Wolczanska 213, 90-924 Lodz, Poland

Abstract

Lately, there are growing concerns over the fate of the wide variety of contaminants of emerging concern (CECs), (e.g. Pharmaceuticals and Personal Care Products (PPCP), Persistent Organic Pollutants (POPs), endocrine disruptors (EDCs), etc.), which are present in effluents, often at trace levels, and often unmonitored. Its extensive usage in medicine, aquaculture and our life, has led to increase CECs concentrations in wastewater. It is known that, water recycling plays a prominent role, especially for water-consuming industries, thus, the purification of wastewaters becomes indispensable to achieve the ideal degree of quality. Limited efficiency of treatment with respect to CECs in conventional wastewater treatment plants (WWTPs) is well known. Many studies showed that Advanced Oxidation Processes could play an important role in removing CECs. Ozone based technologies appear as suitable alternatives since ozone is highly reactive with a broad range of contaminants at room conditions of pressure and temperature. However, low mineralization levels are usually attained since the by-products formed are not prone to further ozone oxidation. Electrochemical advanced oxidation process (electro oxidation and electro reduction, EAOP) and electro coagulation (EC) are two promising techniques that have been used for the abatement of wide variety of organic contaminants. Electrochemical techniques offer the advantage of providing electrons which is a clean, versatile and effective reagent for the elimination of contaminants with high mineralization. Among AOPs, the electro catalytic ozonation processes, combining electrochemistry with ozone is an efficient process due to its simplicity, strong oxidation potential, environment-friendly, and does not require additional reagents.

Plasma Enhanced Chemical Vapour Deposition (PECVD) process leads to the production of the desired layer on the surface of any carrier and is a very versatile method, which falls into the scope of "green chemistry" due to low energy consumption and almost waste-free production process. Plasma polymerization allows for modification of the structure, giving the surface a more hydrophilic character, which is an interesting property for electro catalytic ozonation application and it can lead to better contact between the contaminant and the electro catalyst active sites.

Thus, the introduction of solid electro catalyst and ozone is a cutting-edge approach aiming for water reuse at the lowest cost. The developed solution will be an innovative, modern wastewater treatment with a plasma-based electro catalyst.

The essence of the process is to find both the active, sustained, and photostable plasma-deposited thin-film electro catalysts which enhanced the degradation process with the combined action of ozone. The role of synergistic effects between ozone and plasma-deposited thin film electrode in hybrid electrochemical and ozonation processes of CECs degradation seems to be a key point.

Multiscale Mass Action Law

Miroslav Grmela^{1*}, Abdellah Ajj¹, Jamal Chaouki¹, Vaclav Klika²,
Michal Pavelka³

¹Génie chimique, École Polytechnique, Montréal, Canada,

²Department of Mathematics, Czech Technical University, Prague, Czech Republic

³Mathematical Institute, Charles University, Prague, Czech Republic

Abstract

The classical mass action law is placed into the context of multiscale thermodynamics [1,2,3]. The tools developed in investigations of overall patterns in solutions of governing equations of mechanical systems, as for instance braking the time symmetry, are applied to the governing equations of chemical kinetics. Both the classical mass action law and its extension involving a time reversible part are also lifted to kinetic equations that take into account fluctuations and external forces.

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Keywords

Chemical Kinetics; Multiscale Non Equilibrium Thermodynamics; Contact Geometry

Biography

I have studied in Czech Technical University in Prague; I have PhD in Theoretical Physics from Czechoslovak Academy of Sciences. I have been Professor at École Polytechnique in Montréal. I am interested in Thermodynamics (Equilibrium, Nonequilibrium, Statistical, Chemical), Mechanics of Complex Fluids (Rheology).

Regulation of photosynthesis by the simplest diketone

Shujuan Zhang*

Nanjing University, China

Abstract

The control of harmful algal blooms is a worldwide challenge. Dosing of chemical algicides is a common method in bloom control due to its quick effect and low cost. However, most of the documented chemical algicides lack selectivity and are harmful to non-target organisms. Therefore, considering ecological security and sustainability, the development of eco-friendly algicides is urgently needed. Cyanobacteria are the main species responsible for freshwater algal blooms. Unlike algae and other higher plants, cyanobacteria do not have chloroplasts, and their photosynthetic devices are directly exposed to the cytoplasm, which provides a convenient condition for selective control by regulating photosynthesis. We found that the simplest beta-diketone, acetylacetone (AA), could selectively inhibit the growth of cyanobacteria by regulating the photosynthetic electron transport chain. At the concentration level that is employed for cyanobacterial control, the dosed AA had no harm effects on other aquatic organisms. Given the importance of photosynthesis in both natural and artificial systems, this finding not only provides a unique solution for the selective inhibition of cyanobacteria, but also sheds light on the study of artificial photosynthesis.

Biography

Shujuan Zhang is a full professor in Nanjing University (since 2011). After received her PhD in 2005 from University of Science and Technology of China, she worked as a research associate/postdoc fellow in the University of Hong Kong, National University of Singapore, and Clemson University. She is an editor of Separation and Purification Technology, an editorial member of Journal of Hazardous Materials, and a review editor of Frontiers in Environmental Chemistry. Her current research interests include photochemistry, photocatalysis, photosynthesis, advanced oxidation processes, adsorption and coagulation with focus on the chemistry of water pollution control and environmental functional materials.

Electrically Driven Sic-Based Structured Catalysts for Hydrogen Production

Vincenzo Palma*, Eugenio Meloni, Giuseppina Iervolino
Department of Industrial Engineering, University of Salerno (Italy)

Abstract

1. Introduction

The environmental issues raising from the chemical industry has reached the attention of people all over the world, and the reduction in greenhouse gas (GHG) emissions has been identified as a strategy for the mitigation of climate change. Nowadays, chemical industry is mostly powered by the combustion of fossil fuels, which is responsible for a significant portion of anthropogenic GHG emissions. In this context, many energy experts have agreed that the electrification is the most promising route for reaching the targets, even if electricity generation and transmission involve substantial energy losses and thus its application as a heat source in chemical industry is less efficient than onsite combustion from an energy efficiency point of view. However, the potential of electrification mainly lies in a future scenario where there is a pathway leading to zero-carbon electricity [1]. There are many types of electrification that can be implemented in current chemical industry: power-to-gas (PtG), power-to-chemicals (PtC), power-to-electricity (PtE), power-to-heat (PtH) and power-to-liquids. In the last years, an energy transition has been underway, and many leading energy, transport and industrial companies have taken initiatives to develop the energy transition with hydrogen [2], which is a versatile energy carrier, that can be integrated in different areas such as power grids, transport, heating, fuel-cell electric vehicles, and energy storage . Hydrogen can be produced through different processes, such as natural gas or biogas reforming, gasification of coal and biomass, water electrolysis, water splitting by high temperature heat, photoelectrolysis, and biological processes. Currently, among the above cited processes, the conventional large-scale production of hydrogen is mainly obtained by the reforming of fossil fuels, among which the main processes are methane steam reforming (MSR) and methane dry reforming (MDR). The two mentioned processes are highly endothermic; therefore, the constant supply of heat to the catalytic sites is one of the main constrain limiting their efficiency. In these reactors huge temperature gradients occur from the reactor external side to the catalyst bed, due to the heat transfer resistance mainly linked to the low thermal conductivity of the commercial catalysts actually used [3]. In this work the process intensification of both MSR and MDR is proposed by using an innovative structured catalyst which combines two fundamental features (i) a high thermal conductivity, that aim to flatten the thermal profile inside the reactor , and (ii) an integrated joule heating, that allow to perform a direct electricity-driven process. In this way, the energy is directly supplied to the catalyst, due to its intimate contact with the electric heat source, therefore the removal of thermal limitations and a better control of the reaction front may be obtained.

2. Methods

In this work a laboratory-scale reactor has been realized, using a commercial silicon carbide (SiC) electrical heating element that simultaneously acted as heating medium and support for the catalyst. In this way, the sense of the heat flux has been inverted (from the center to the external) with respect to the conventional reformer (from the external to the center). Commercial ceramic material was employed as support for the Ni-based catalysts preparation. A fixed amount of 5 wt% Ni was deposited on the support, previously dried and calcined at 850 °C in air. The catalysts were prepared via wet impregnation, with a solution of Ni(NO₃)₂·6H₂O as Ni precursor; the resulting catalysts were dried at 120 °C for 2 h and calcined at 850 °C in air for 1 h. The catalysed SiC element has been enclosed in a properly shaped quartz reactor and a mixture consisting of 10 vol% of CH₄, 30 vol% of Steam and diluted in argon has been fed from the top to the bottom of the reactor. As regards the preliminary electrified MDR tests carried out on Ni catalysed SiC element, the same reactor configuration described in the previous paragraph was used. In particular, a mixture consisting of 50 vol% of CH₄ and 50 vol% of CO₂ has been fed to the reactor.

3. Results and Discussion

The results of the preliminary MDR test evidenced that the methane conversion and hydrogen yield (Figure 1) are particularly promising. In particular, it is possible to observe that the catalytic SiC element is able to reach the reaction temperatures by means of the Joule heating. It is possible to note that the MDR reaction proceeds following the equilibrium thermodynamic profile of the reaction (black curve) even at low temperatures.

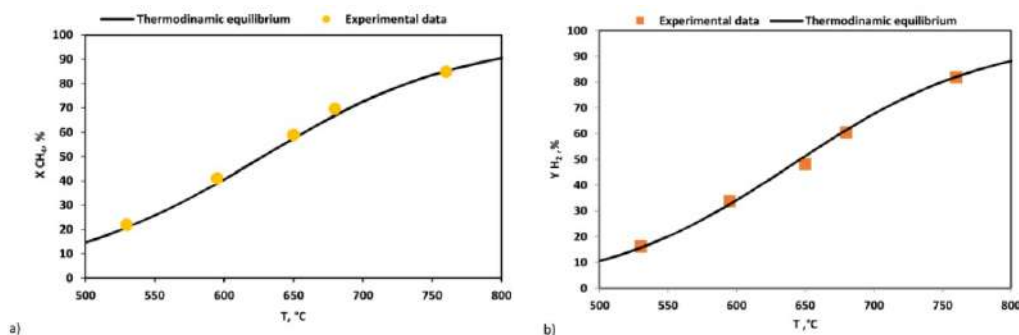


Figure 1. catalytic activity test results (MDR) a) CH₄ conversion; b) H₂ yield; CO₂/CH₄ ratio for MDR reaction = 1; WHSV = 70 h⁻¹.

As expected, the energy consumption of the system is strictly linked to the H₂ productivity; in fact, the higher is this amount the lower is the energy consumption. Moreover, at lab scale, the effects of heat dissipation have a big role with respect to the low gas flow rate fed to the reactor and for this reason higher energy consumption was observed at the lower WHSV values. The direct comparison in terms of energy consumption for H₂ production with other electrified reforming processes is very difficult, since not a so high number of data is available in literature. However, from preliminary results, it is possible to confirm that energy

consumption values close to that reported for other electrified processes, including the modern electrolysers,

4. Conclusions

The results reported in this work demonstrate that a commercial SiC based heating element, coated with a Ni-based catalyst, can be used in the context of the chemical processes electrification scenario, a topic that is acquiring more and more focus from the scientific and industrial world. The investigation concerning the adoption of the Ni catalysed SiC electrically heated element pointed out its effective capacity of heating up the reaction zone without any external source till temperature of 900 °C. It is possible to summarize that the results have shown values close to that reported for other electrified processes, including the modern electrolysers. These results can be considered even more promising if one takes in to account the laboratory scale of the reactor, where the effects of heat dissipation have a big role with respect to the low gas flow rate fed to the reactor.

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Biography

Vincenzo Palma, (Industrial Chemist) Full professor of Industrial Chemistry and Nanostructured catalysts for Energy and Environment at the University of Salerno – Italy. Since the Degree Thesis, his research has been carried out in the field of catalytic processes applied to the energy production and pollution control. More recently, some of his activities considered the application of microwaves to heterogeneous catalysis for the assisted regeneration of catalytic filters for the abatement of carbon particulate and also for the intensification of endothermic system. During the years, the study also addressed the membrane assisted catalytic conversion processes of hydrocarbons for the production of hydrogen, with particular attention to the autothermal reforming processes of light hydrocarbons and to the low temperature steam reforming of ethanol. Pollution Control: Catalyzed wall flow monolith for the microwave assisted DPF regeneration Low temperature hydrolysis catalysts for the COS abatement. Process intensification: Microwave susceptible structured catalysts for the distributed hydrogen production Catalytic oxidative decomposition reaction of H₂S for the simultaneous production of Sulphur and H₂ High thermal conductivity catalysts for the CO-WGS process intensification



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Poster Presentation

Autodisplay of the Saccharase SacA from *Bacillus Subtilis* in *E. Coli* for Whole Cell Biocatalysis

Jorge Sánchez Andrade¹, and Antonio De Leon-Rodriguez^{1,*},

¹División de Biología Molecular, Instituto Potosino de Investigación Científica y Tecnológica, A.C., Camino a la Presa San José 2055, Col. Lomas 4^a Sección, C.P. 78216 San Luis Potosí, SLP, México.

Abstract

The goal of this work was the use of the auto-transporter Adhesin Involved in Diffuse Adherence (AIDA) from *Escherichia coli* to express on the bacterial surface the saccharase SacA from *Bacillus subtilis* to carry out whole cell biocatalysts and hydrolysate sucrose in *E. coli*. For this, pAIDA-SacA vector was designed and constructed guided by the preferred codons to be expressed in *E. coli*. Restriction assays and DNA sequencing confirmed molecular construction. Then DH5a cells were transformed and enzyme activity was corroborated using sucrose as substrate in agar plates. The optimal conditions for the biocatalyst were temperature of 45°C and pH 4.5. Then the plasmid was used to transform genetically engineered *E. coli* strains to produce metabolites such as ethanol, and organic acids from sucrose. Results demonstrate that the designed pAIDA-SacA vector has the ability to express active sucrose to carry out whole cell biocatalysis. Biocatalyst can be used hydrolysate sucrose for several biotechnological applications such as biofuels and other metabolites production. Acknowledgments: Partial funding through the Grant CONACyT 281700.

Keywords

Autodisplay; Sucrose; Saccharase; Whole-Cell Biocatalyst

Biography

Antonio De Leon Rodriguez studied his Bachelor Science on Chemical Science and he got the award “To the best student of Mexico”. He studied a Master in Biotechnology at National Autonomous University of Mexico, on the recombinant protein expression, and obtained the degree with honors and the award for “The best thesis on engineering” by the Mexican Academy of Engineering. PhD was made in the same Institution, on culture of human hematopoietic cells in bioreactors and received the prize “Alfonso Caso” for his doctoral thesis. He performed an academic stay in the Department of Genetics at the University of Cambridge, UK.



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