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ABSTRACT BOOK

7th International Conference on

CATALYSIS AND CHEMICAL ENGINEERING

February 20-22, 2023 | **Las Vegas, NV**

February 23-24, 2023 | Online

Venue:
Hampton Inn Tropicana
4975 S. Dean Martin Dr.
Las Vegas, Nevada, USA

Timezone:
Pacific Time

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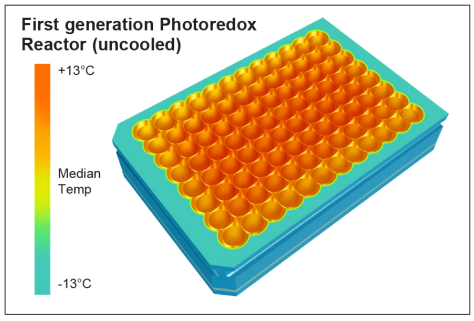

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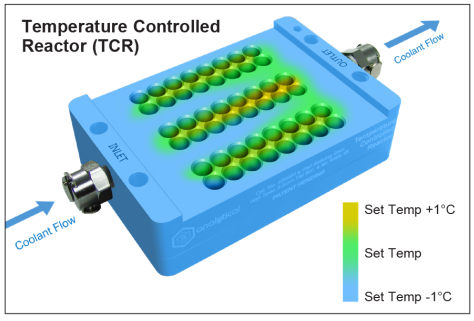

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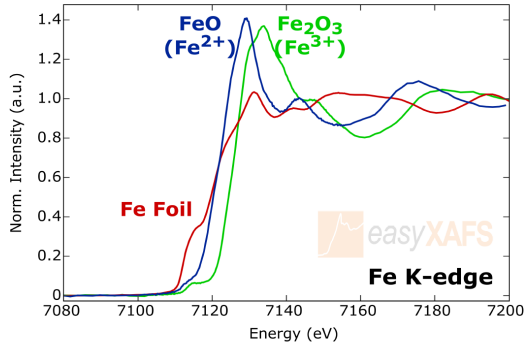

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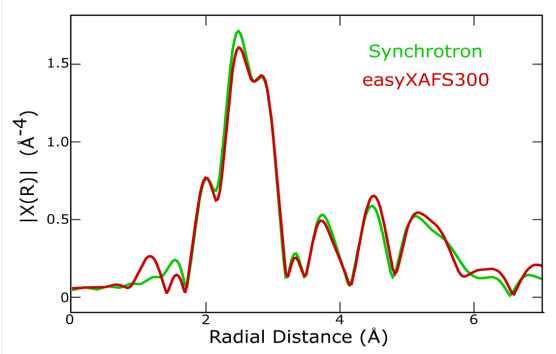

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BELSORP MAX X Features

- **Specific surface area range:**
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  - 0.0005 m^2/g or more (Kr)
- **Pore size distribution range:**
  - 0.35 to 500 nm
- **Highly accurate vapor adsorption measurement under strict temperature control**
- **Advanced GCMC / NLDFT method offers higher resolution & more precise PSD analyses**
- **IoT: Measurement status & results are sent remotely via e-mail notification system**

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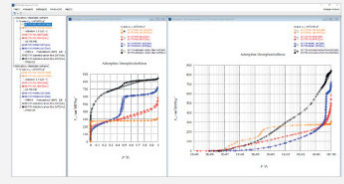
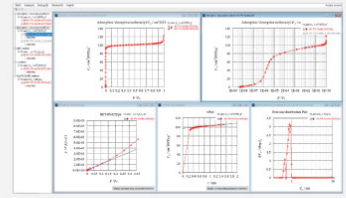
For inexperienced users or for measurements of unknown samples, BELCONTROL only requires basic sample information (name, mass, etc.), pre-treatment conditions (if not performed externally) and the measurement range. Detailed control of the configuration and measurement settings is possible to optimize the measurement conditions (e.g. dosing settings, equilibrium criteria, leak test option, etc.). This allows the user to fully customize the sample analysis to his needs.

- Analysis data and results can be saved by Drag & Drop (MS Excel format)
- Easy change of chart overwriting, X-Y axis scaling, unit conversion, point markers and color
- Analysis results window can be saved for further analysis after a computer restart
- Equipped with a routine analysis setting function, useful for performing the same analysis every time
- Customized data can be registered as standard reference isotherms in pore profile analyses, t-plot and αs
- Improved visibility for different analyses through individual color setting for custom data



Isotherms starting from relative pressure of approx. 10^{-9}



Analysis results: Isotherm, BET (according to ISO 9277), t-plot and pore size distribution by GCMC

TECHNICAL INFORMATION

Measurement principle		Volumetric method + AFSM™ (Advanced Free Space Measurement)
Adsorption gas		N_2, Ar, Kr, CO_2, H_2, O_2, CH_4, NH_3, NO, CO, butane, and various other (non-)corrosive gases
Adsorption vapor		H_2O, MeOH, EtOH, C_6H_6, CCl_4, hexane, and various other (non-)corrosive vapors
Number of measurements (high accuracy mode)		Max. 4 ports simultaneously (3)
	Specific surface area	0.01 m^2/g~ (N_2), 0.0005m^2/g~ (Kr) (depending on sample density)
	Pore size distribution (ø)	0.35~500 nm
	Low pressure isotherm	$P/P_0 \approx 10^{-9}$ ~ (N_2 @ 77K, Ar @ 87K)
	Vapor adsorption	P/P_0 = ~ 0.95 @ 40°C
Pressure transducer	**133 kPa (1000 Torr)**	6
	1.33 kPa (10 Torr)	4 (max.)
	0.0133 kPa (0.1 Torr)	3 (max.)
Thermostatic air oven		50°C
Gas ports		3 ports * (optional: 6.9 or 12 ports max.)
CE certificate		✓

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Microtrac Inc.
3230 N. Susquehanna Trail
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Tel.: +1 888 643 5880
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MicrotracBEL Corp.
8-2-52 Nanko Higashi, Suminoe-ku
Osaka 559-0031
Japan

Tel.: +81 6244 34393
sales@microtrac-bel.com
www.microtrac.com

Microtrac Retsch GmbH
Retsch-Allee 1-5
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Moderator Presentation

Catalytic Potentials of Metal Complexes Supported on Chloromethylated Polystyrene Cross-Linked with Divinyl Benzene

Mannar Ram Maurya

Indian Institute of Technology Roorkee, India

Abstract Not Available!!!

Plenary Presentations

Model Systems for Heterogeneous Catalysts at the Atomic Scale: Can Surface Science Contribute?

Hans-Joachim Freund

Fritz Haber Institute, Germany

Abstract Not Available!!!

Surfaces as Ligands, Activators, and Catalytic Models for Polyolefin Construction and Deconstruction

Tobin J. Marks

Northwestern University, Evanston, IL

Abstract Not Available!!!

Grand Canonical Quantum Mechanics with Applications to Mechanisms and Rates for Electrocatalysis

William A. Goddard III

California Institute of Technology, Pasadena, CA

Abstract Not Available!!!

Catalytic Coupling of Methane and CO2 to Produce Higher Oxygenates

James J. Spivey

Louisiana State University, Baton Rouge, LA

Abstract Not Available!!!

Nobel Presentation

Thermally Stable Single Atom Catalysts

Yong Wang

Washington State University, Pullman, WA

Abstract Not Available!!!

Keynote Presentations

How Olefin Metathesis Catalysts Form from Olefins, and More

Richard R. Schrock

Massachusetts Institute of Technology, Cambridge, MA

Abstract Not Available!!!

New Insights on the Impact of Geometrical and Electronic Structure in Water Oxidation Catalysis

Craig L. Hill

Emory University, Atlanta, GA

Abstract Not Available!!!

Plasmonic Catalysis: Thermal plus Nonthermal for Maximum Light Enhancement

Zhijia Geng
Yifan Yu
Joey Offen
Jie Liu*

Department of Chemistry, Duke University, Durham, NC

Abstract

In plasmonic catalysis, recent studies have shown that both photothermal effect and hot-carrier-based nonthermal effect are important for the overall enhancement of reaction speed by light. Our group have developed method to experimentally untangle the thermal and nonthermal effects, which contributed significantly to the development of more accurate understanding of plasmonic catalysis. More recently, it became obvious that the combination of both thermal and non-thermal effects was the most effective approach to maximize the effect from light. Nonthe-less, the net results from plasmonic catalysis should be a greatly enhanced reaction speed, regardless of whether the main factor is thermal or nonthermal. IN this presentation, a system study on how to optimize the overall light efficiency in plasmonic catalysis will be presented and the potential application for a full spectrum photocatalysis process will be discussed.

Biography:

Jie Liu is the George B Geller Professor of Chemistry at Duke University. He earned a B.S. in Chemistry from Shandong University in 1987 and a Ph.D. in Chemistry from Harvard University in

1996. His research interests include synthesis and chemical functionalization of nanomaterials, plasmonic catalysis, nanoelectronic devices, scanning probe microscopy, and carbon nanomaterials. He is elected as a Fellow in AAAS (2013), APS (2014) and RSC (2013). He also serves as an associate editor for RSC journal Nanoscale between 2012 and2018. He is currently an associate editor for Nano research since 2018.

A New Class of Adamantyl Based Bidentate Ferrocenyl Phosphine Ligands (Mphos) and Catalysts for the Synthesis of API Molecules via Csp2-Csp3Cross Couplings

Thomas J. Colacot

MilliporeSigma, Milwaukee, WI

Abstract Not Available!!!

Thermostability, Tunability, and Tenacity of RNA as Motile and Dynamic Polymeric Materials in Nanotechnology and Nanomedicine

Peixuan Guo

The Ohio State University, Columbus, OH

Abstract Not Available!!!

New Nanostructures for Increased Selectivity and Stability in Catalysis

Francisco Zaera

University of California, Riverside, CA

Abstract Not Available!!!

Comparative Studies of Fe and Co-Based Core-Shell Catalysts for Fischer-Tropsch Synthesis in SS Microreactors

Debasish Kuila

North Carolina A&T State University, Greensboro, NC

Abstract Not Available!!!

Oral Presentations

Conformationally Locked *cis*-1,2-Diaminocyclohexane-based Chiral Ligands for Asymmetric Catalysis

Carim van Beek[1]*
Vyachslav V. Samoshin

University of the Pacific, USA

Abstract

An efficient synthesis for a new conformationally locked chiral *cis*-1,2-diaminocyclohexane scaffold has been developed. The conformational lock allows for convenient symmetrical derivatization of the amino groups through the reductive amination strategy. A series of optically pure chiral ligands based on the *cis*-DACH scaffold has been generated to demonstrate a proof-of-concept for these ligands as chiral catalysts in the asymmetric Henry reaction. Excellent yields with moderate enantioselectivity were demonstrated at room temperature, with an increase in enantioselectivity at lower temperatures, showing the potential of this new type of *cis*-DACH ligand.

Biography

Highly motivated scientist with a background in organic synthesis, currently working in the pharmaceutical industry. Received a Bachelors' and Masters' in chemistry in the Netherlands, then moved to California, USA for a PhD in Pharmaceutical and Chemical Sciences. My PhD research was focused on developing novel ligands for asymmetric synthesis, chiral resolution of synthetic intermediates, and enzymatic catalysis methodologies. My current activities involve the chemical development of APIs at Kronos Bio, to support clinical trials, regulatory filings, and future commercialization of pipeline drugs. Activities include process development for drug substance, managing CROs/CMOs, and selecting, and developing regulatory starting materials.

Reaching Saddle Points of Complex Potential Energy Surfaces using ARTn-DFT

Anne Hemeryck *

LAAS-CNRS, Université de Toulouse, CNRS, Toulouse, France

Abstract

In surface catalysis, the evolution of many systems is determined by activated mechanisms that occur on a wide range of time scales. To help predict the performance of materials for catalysis, numerical methods must be able to search for and identify these events with the goal of reproducing the energy surface and tracking the evolution of these systems at the atomic level on time scales from nanoseconds to seconds and beyond.

In this talk, I will present an alternative method combining the Activation Relaxation Technique nouveau (ARTn) with ab initio (DFT) software for the calculation of interatomic forces along the reaction path. This method differs from other currently known methods by its efficiency in finding and identifying chemical reactions occurring at the atomic scale in complex systems and by its ability to find reaction mechanisms without prior knowledge of the atomic positions of the final product. In this presentation, I will present the ARTn-DFT coupling and its application on chemical reactions on the oxide surface.

Biography:

Anne HEMERYCK is a researcher at LAAS-CNRS in Toulouse France. She is the Head of the Multi-levels Modeling of Materials research team and she is also the deputy director of the MicroNanoBioTechnology department in LAAS-CNRS. Her research activities focus on the development of multi-levels computational methods (from ab initio to mesoscale techniques), dedicated to physical and chemical problems in material science, notably on the predictive simulation of materials in microelectronics fields. She addresses a wide range of application in nanotechnologies with a particular focus on atomic diffusion at surface and interface (defects diffusion, detection mechanism...).

Adsorption and advanced oxidation of pharmaceuticals and their toxic byproduct formation potentials in water by graphene oxide-complex metal oxide composites

Wei-Hsiang Chen*
Yu-Chun Tseng
Shih-Wen Peng
Kai-Lin ChenMing-Chuan Ho
Yu-Ting Huang
Jhang-Ruei Huang
Chi-Min Li

Institute of Environmental Engineering, National Sun Yat-sen University, Taiwan

Abstract

Graphene oxide (GO) is hydrophilic and possesses a large surface area. It is an adsorbent to remove contaminants from aqueous solutions, with the potential of enhancing the degradation of compounds through the advanced oxidation process (AOP). Pharmaceuticals have been detected in the environment repeatedly and are known to be difficult to remove in conventional treatment technologies. Several pharmaceuticals of concern were selected as the targets in this study. For example, acetaminophen (Apap) is a medication widely used and its usage is expected to be increased significantly during the COVID-19 pandemic. Various GO-complex metal oxide (GO-XY_2O_4) composites were synthesized by co-precipitation using the combination of different metals such as Fe^{2+}, Co^{2+}, Ni^{2+}, and Fe^{3+}. This study investigated the adsorption and catalytic degradation of acetaminophen and other pharmaceuticals in batch experiments by applying these GO-XY2O4 composites as the adsorbents or catalysts, with different substances including persulfate and hydrogen peroxide being added as the oxidant to activate the AOP. The surface property of the composite, effects of the initial pharmaceutical concentration, catalyst composition, type and concentration of oxidant, reaction pH, and reaction time on the treatment performance were discussed. In addition, certain pharmaceuticals form toxic byproducts during chlorination. The feasibility of employing these GO-XY_2O_4 composites for reducing the formation potentials of these toxic byproducts was also discussed.

Biography:

Wei-Hsiang Chen is a professor at the Institute of Environmental Engineering at National Sun Yat-Sen University (NSYSU) in Kaohsiung of Taiwan. He is also the Associate Director of the Aerosol Science Research Center at NSYSU. Dr. Chen received his Ph.D. degree in Environmental Engineering from the Department of Civil and Environmental Engineering at UCD in 2009. His research interests focus on environmental chemistry and microbiology, water and wastewater treatment technology, emerging contaminants and disinfection byproducts, multi-media environmental fate, transport, and distribution, and health risk assessment.

Global Optimization and Large-Scale Molecular Simulations for Catalysis Problems

Vassiliki-Alexandra Glezakou

Oak Ridge National Laboratory, Oak Ridge, TN

Abstract Not Available!!!

Direct CO2 Hydrogenation to Aromatics Over Bifunctional ZnZrOx/ZSM-5: Effect of Zeolite Morphology to Product Distribution

Mansoor Ali*
Faisal Zafar
Jong Wook Bae

School of Chemical Engineering, Sungkyunkwan University (SKKU), Republic of Korea

Abstract

The increasing demands of CO2 reduction to mitigate its adverse impacts on environment have forced to develop the catalytic conversions of CO2 to synthesize value-added chemicals and clean fuels. Among the synthesized hydrocarbons, alkylated aromatic fractions are considered as the most valuable chemicals. The concepts of bifunctional catalysis by combining metal oxides as active sites for CO2 hydrogenation to methanol and solid acid catalysts to convert methanol into aromatics have been largely investigated. Especially, ZSM-5 with MFI topology, well-designed channel structures and adjustable acid sites has been regarded as the preferred catalytic systems for direct aromatics production from CO2. Besides the zeolite topology, the zeolite morphologies play crucial roles to tune the aromatic distributions by changing diffusion rates of reactants and products as well as acidic properties. The present study is focusing on the effects of morphology of various ZSM-5 zeolites (N-ZSM-5, HN-ZSM-5, SL-ZSM-5 and C-ZSM-5) to CO2 hydrogenation activity and hydrocarbons distributions on the bifunctional catalysts by adjusting the surface properties according to different morphologies of HZSM-5 zeolites. The bifunctional ZnZrOx hybridized with different morphologies HZSM-5 (ZnZr/ZSM-5) exhibited different catalytic activity and product distribution with maximum CO2 conversion and aromatic selectivity with reasonable CO selectivity on the ZnZr/N-ZSM-5. On the bifunctional ZnZr/ZSM-5 catalysis, the variations of ZSM-5 morphologies largely changed the physicochemical properties (porosity, particle size and acidic site) of the various ZSM-5 zeolites. The morphologies of ZSM-5 were responsible for an increased activity and aromatics due to enhanced diffusion rates as well as abundant stronger Brønsted acid sites.

Biography:

Mansoor Ali received his B.E. degree in Petroleum and Natural Gas engineering at Mehran University of Engineering and Technology, Pakistan, in 2014. From March 2015, he worked as a trainee petroleum engineer at KUFPEC (Kuwait Foreign Petroleum Exp. Co.) for one year. In 2016, he was awarded the scholarship for higher studies by HEC (Higher Education Commission) Pakistan. Since September 2016, he is a Ph.D. student in the group of Prof. Jong Wook Bae at School of Chemical Engineering, Sungkyunkwan University (SKKU), South Korea. His research mainly focuses on the development of heterogeneous bifunctional catalysts for CO2 hydrogenation to aromatics.

Poster Presentations

Different hybrid formation aspect of numerous tiny-sized carbon nanofibers in carbon-based nonwoven fabrics with or without the cyclic process

Hyun-Ji Kim
Sung-Hoon Kim*

Department of Engineering in Energy & Applied Chemistry, Silla University, Republic of Korea

Abstract

Carbon microcoils (CMCs) were formed in carbon-based nonwoven fabrics (c-NFs) under C_2H_2 + SF_6 gas flow in a thermal chemical vapor deposition system. The incorporation of H_2 gas flow into the C_2H_2 + SF_6 gas flow system resulted in the selective hybrid formation of numerous tiny carbon nanofibers (CNFs) only on the surfaces of the individual carbon fibers (i-CFs) in the c-NFs, not on the surfaces of the CMCs. This selective formation of tiny CNFs is ascribed to the different intrinsic material characteristics of the CMCs and i-CFs. Systematic diagrams are presented that explain how the incorporation of H_2 gas flow into the C_2H_2 + SF_6 gas flow system causes the selective hybrid formation of numerous tiny CNFs. The nonselective hybrid formation of numerous tiny CNFs on the surfaces of both the i-CFs and CMCs in c-NFs was achieved using a cyclic process in the C_2H_2 + SF_6 + H_2 gas flow system. The production of a larger number of smaller Ni catalysts caused by the abundant C_2H_2 gas environment during the reaction appeared to be the main cause for this nonselective hybrid formation. Furthermore, increasing the number of SF_6 on/off cycles in the cyclic process increased the number of tiny CNFs that formed on the surfaces of the CMCs because it maintained the smaller Ni catalysts on the CMC surfaces. Systematic diagrams are presented that explain both the nonselective formation of numerous tiny CNFs by the cyclic process and the increase in the number of tiny CNFs on the surfaces of the CMCs with increasing number of SF_6 on/off cycles in the cyclic process.

Biography:

Sung-Hoon Kim is a renowned materials chemist who has largely influenced his field and directly aided in the development of new chemical synthesis methods and nanomaterials. Dr. Kim received a Ph.D. in Chemistry in 1993 from Seoul National University in South Korea and additionally earned another Ph.D. in Advanced Electronics & Optical Science in 2005 from Osaka University in Japan. From 1988 to 1998, he was a Senior Researcher in the New Materials Laboratory of Samsung Advanced Institute of Technology (SAIT). Since 1998, Dr. Kim has been a Full Professor at Silla University in South Korea.

Complete Photocatalytic Decomposition of Malodorous gas using MOFs Composites as Visible-light Photocatalyst

Suho Kim*
Minhyung Lee
Hyoung-il Kim

Department of Civil & Environmental Engineering, Yonsei University, Republic of Korea

Abstract

Methyl mercaptan (CH_3SH) is a kind of typical volatile organic sulfur compounds (VOSCs) generated from sewage treatment works, wood-pulping industry, and energy-related activities. Methyl mercaptan has a highly low olfactory threshold of 2 ppb, which could have a toxic effect on humans and the natural environment. It is fatal to human health, ranging from skin irritation, respiratory paralysis, and even death due to prolonged exposure.

Copper-based metal organic frameworks (MOFs) doping with Ag_2O composite was successfully synthesized and applied for the removal of gaseous methyl mercaptan. Ag_2O@Cu-MOFs completely decomposed methyl mercaptan under visible light irradiation at room temperature without the formation of intermediate gas from methyl mercaptan or toxic sulfur-based compounds. By impregnation of Ag_2O, specific surface area of Ag_2O@Cu-MOFs was 830.1 m^2g^{-1}, which was 16 times that of Cu-MOFs. It was verified that the surface reaction of photocatalyst composite was activated by forming hierarchical micropores after doping Ag_2O. In addition, it was demonstrated that the light absorption in the visible light spectrum was increased by Ag_2O, and that the recombination of electrons and holes was inhibited. Unlike Cu-MOFs, complete

mineralization of methyl mercaptan was stoichiometrically achieved converting to carbon dioxide by Ag_2O@Cu-MOFs and visible light irradiation.By performing complete photo-oxidation of sulfur-based odor substances in the visible light region at room temperature without the formation of intermediate products or toxic sulfur compounds, a new direction could be suggested for advancement of malodorous removal technologies.

Biography:

Suho Kim Living in the Seoul metropolitan, I also experienced significant changes in the quality of life, which was indexed on the air quality. I realized that contributing to pollution management is as important as contributing to any other field of Science & Technology. So, I worked on the application of materials in energy and environment and I am looking for an opportunity to diversify my interest in the field and devise edge-cutting technologies for air pollution mitigation. So far, I have published 16 SCI-indexed research papers in reputed journals with 4 patents and 3 technology transfers.

Multicomponent antimonide as efficient and low-cost catalysts

Terje Finstad[1]*
Nayereh Soltani[1]
Jamil Ur Rahman[2]
Patricia Almeida Carvalho[3]

[1]University of Oslo, Norway
[2]Leibniz Institute Dresden, Germany
[3]SINTEF, Norway

Abstract

Multicomponent intermetallic compounds consisting of different transition metal elements with high/medium configurational entropy could be ideal candidates for catalysts in complex reactions. The possibility of electronic modification and isolation of active sites along with the structural stability in these compounds can result in excellent catalytic properties. Herein, we report a series of single-phase quinary antimonide intermetallic compounds with the chemical composition of $(NiCoFeCu)_{1-x}Sb_x$ which has a NiAs type crystal structure from bulk to nanoscale. The nanosized samples were synthesized using both top-down and bottom-up approaches through ball milling and thermal treatment method, respectively. The catalytic performance was examined in the hydrogenation of *p*-nitrophenol to *p*-aminophenol using $NaBH_4$. Structural and morphological characteristics of the synthesized samples before and after 10 runs of catalytic performance are described in detail. The kinetic rate constant for the best synthesized sample (Nano40) is about 10-times higher than that for the synthesized bulk sample. All synthesized samples exhibit improved catalytic activity and extreme durability during the reaction compared to the bimetallic nanoscale catalyst in the NiAs type structure. This report on heterogeneous catalysis demonstrated that the catalytic activity is drastically enhanced and could be beneficial for creating novel high-performance catalysts making the multicomponent structures attractive alternatives to noble metal based catalysts.

Biography:

Terje Finstad is a full professor in physics at the University of Oslo since 1985. He has worked at Bejing Institute of Technology, Middle East University in Turkey, University of Minneapolis, Bell Communication Research Lab, University of North Carolina, California Institute of Technology and Defence Research Lab in Norway within materials science and nanotechnology.

Effect of Mg-incorporation in sodium promoted magnetite during CO_2 hydrogenation.

Jaehoon Kim[1,2,3]*
Sheraz Ahmed[3]
Muhammad Kashif Khan[1,2]
Muhammad Irshad[2]
Yoon Woonjong[3]

[1]School of Chemical Engineering
[2]School of Mechanical Engineering
[3]SKKU Advanced Institute of Nano Technology, Sungkyunkwan University, South Korea

Abstract

The attractive and considerable approach of CO_2 hydrogenation into higher hydrocarbons is the significant route to utilize CO_2 as a part of large-scale industrial processes. However, the design of a highly selective and active catalyst is a great challenge due to the high energy barrier of CO_2 molecule. Herein, we present bimetallic sodium-promoted iron magnesium oxide (Na-FeMgO$_x$) catalyst that is effective for producing a high C_{5+} yield of 25.1% at a CO_2 conversion of 49.1%. The magnetite (Fe_3O_4) phase which is considered as surface oxygen vacancy to facilitate the reverse water-gas-shift (RWGS) reaction to form CO, whereas the Hägg iron carbide (χ-Fe_5C_2) phase facilitates C–C coupling for hydrocarbon production. The electronic behavior of Mg helps to convert iron-based catalysts to iron carbide to facilitate the Fischer-Tropsch reaction; and the magnetite behavior of bimetallic Na-FeMgO$_x$ catalyst enhanced CO_2 and H_2 adsorption, which facilitate the formation of carbonate, bicarbonate, and formate species via the RWGS reaction. The Mg promoter helps to enhance the hydrocarbon selectivity and suppress methane formation, demonstrating its practical application in a large-scale industrial process. Furthermore, the deactivation behaviour of magnesium-based catalysts was explained for the first time, in which active and inactive phase segregation and positioning towards the surface were investigated in detail based on HR-TEM and HAADF.

Biography:

Jaehoon Kim received his Ph.D. in Chemical and Biomolecular Engineering from North Carolina State University in 2005 on the topic of thin film deposition using liquid and supercritical carbon dioxide. He then worked as a National Research Council research associate at U.S. Army Research Office from 2005–2007 and as a senior scientist at Clean Energy Research Center at the Korea Institute of Science and Technology from 2007–2013. Since 2013, he has been a professor at the School of Chemical Engineering, School of Mechanical Engineering, and SKKU Advanced Institute of Nano Technology at Sungkyunkwan University. His research focuses on nanoscale energy conversion and energy storage materials, biofuels and biochemicals, CO2 conversion to liquid fuels and chemicals, separations, and supercritical fluid technologies. He has been authored and co-authored in more than 200 peer-reviewed journal articles and more than 55 patents. He serves as a subject editor of Korean Journal of Chemical Engineering, and as editorial board members of Energy Science & Engineering, Journal of Supercritical Fluids, Catalysts, and Biomass.

Energy Harvesting from Water Potential Gradient Using Porous Diatomite by Adding Carbon Black

Pei-Cheng Tsai
Ruey-Jen Yang*

Department of Engineering Science, National Cheng Kung University, Tainan, Taiwan

Abstract

Energy is one of the most important social issues nowadays. Inspired by the evaporation in the water cycle, this study uses evaporation as the driving force of water to design an upright experimental device (EDPG) which is composed of gypsum, diatomite and carbon black. The results show that EDPG can stand alone in deionized water (DI water), the maximum output power of a single EDPG can reach 7.73 nW. Also, due to the Ionovoltaic effect, the water level of the experimental device (EDPG), the ion flow in the channel and the electrode position have a significant impact on its power generation mechanism. Finally, by adding lithium chloride (LiCl) into EDPG, the electrical response is highly sensitive to the humidity change on both sides of EDPG. The short circuit current can reach about 150 nA under the situation (the relative humidity difference is 60 %). Through this study, we can understand the potential of EDPG as an evaporative generator, and it is expected to develop into high-efficiency devices that can generate electricity and dehumidify at the same time in the future.

Biography:

Yang has worked in industry in the USA for over 10 years after receiving his Ph.D. from the University of California at Berkeley in 1982. Professor Yang joined the National Cheng Kung University since 1993 and currently is a Chair Professor and a research fellow of the Taiwan Ministry of Science and Technology. He is also a fellow of the American Society of Mechanical Engineers (ASME) and Society of Theoretical and Applied Mechanics (STAM). His research focuses on Fluid/Thermal Sciences, Microfluidics, Nanofluidics, and Energy Conversion.

Immobilization of photocatalyst TiO2 on rubber tiles and photocatalytic wind tunnel design for treatment of polluted air: Croatian case study

Marija Tomaš*
Paula Benjak
Lucija Radetić
Ivana Grčić

University of Zagreb, Faculty of Geotechnical Engineering, Croatia

Abstract

Solar photocatalysis has been proven as a promising technology for air purification for real scale applications. One of the most researched photocatalysts, titanium dioxide (TiO_2) irradiated with UV light, can decompose many organic compounds to water, carbon dioxide, and mineral acids or their salts Nowadays, a variety of reactors and methods of photocatalyst immobilization have been proposed for air treatment. Rubber tiles as an existing product from recycled rubber (floor covering and cast rubber) were immobilized with commercially available TiO_2 P25 by sol-gel method in order to get photocatalytic active layer on the product surface. The photocatalytic wind tunnel is a custom-made reactor designed by the principles of a wind tunnel with the blower. The whole construction was adjusted to the test chamber in order to achieve simulation of an outdoor environment.

Therefore, in this work, we are presenting photocatalytic wind tunnel (PWT) as the reactor for testing photocatalytic degradation of airborne pollutants by TiO_2-immobilized on rubber tiles. Immobilization was validated by SEM-EDS and FTIR analysis. The stability and environmental impact of PRT were investigated by leaching test and AAS and TOC analyses. The results of the leaching test are compared with the Ordinance on the methods and conditions for the landfill of waste, categories, and operational requirements for landfills and the Toxicity Characteristic Leaching Procedure (TCLP).

Biography:

Marija Tomaš works as an assistant at the project „Recycled rubber & solar photocatalysis: ecological innovation for passive air and health protection" at the University of Zagreb. Her research interests as a PhD student of Environmental Engineering focus on solar photocatalysis, air purification, reuse of waste materials for photocatalysis and the preparation of catalysts.

Methods of Immobilization of Titanium Dioxide on Rubber Tiles Made from Recycled Tyres for Passive Air Protection by Solar Photocatalysis

Paula Benjak

University of Zagreb, Croatia

Abstract Not Available!!!

Highly efficient catalysts for industrial flue gas desulfurization and resource utilization

Yao Lu[1]*
Qijie Jin[1,2]
Haitao Xu[1,2]

[1] School of Environmental Science and Engineering, Nanjing Tech University, Nanjing 210009, PR China
[2] Nanjing Gekof Institute of Environmental Protection Technology & Equipment Co., Nanjing 210031, PR China

Abstract

Coal-fired flue gas is the main source of sulfide emissions. High sulfur content in coal, coal combustion will produce a lot of SO_2 and COS. In recent years, with the rapid development of electric power and steel industry, the annual consumption of coal increases year by year, and the total emission of sulfide also increases. At present, the desulfurization process widely used at home and abroad has high desulfurization efficiency and stable operation, but the by-product utilization rate is low, occupies a large amount of land, and easily causes secondary pollution. Efficient removal and resource utilization of sulfides become research focus.

A series of catalyst systems for catalytic reduction of SO_2 to sulfur with CO were studied. The results showed that 15% La-Ce-O_x@ZrO_2 catalyst had the best activity. When the reaction temperature is 350 °C, the SO_2 conversion rate is 100%, the S yield and S selectivity are both greater than 96%. The ZrO_2 as a carrier reduces the acidity of the catalyst and improves the weak basic sites of the catalyst, which is beneficial to the adsorption and activation of SO_2 molecules at low temperature. The incorporation of La and Ce increased the oxygen concentration adsorbed on the catalyst and improved the activity of the catalyst. The main reaction intermediates were

weakly adsorbed SO_2(SO_3^{2-}), bicoordinated CO_3^{2-}, monodentate carbonate and CO in the gas phase. Therefore, the catalytic reaction followed both L-H and E-R mechanisms.

Biography:

Yao Lu was born in Jiangsu, China, in 1998. He is currently pursuing his master's degree in College of Environmental Science and Engineering of Nanjing Tech University with the supervision of Professor Haitao Xu. He has published three research papers in peer-reviewed journals. He has two granted Chinese invention patents. His research interests focus on the environment catalysis, mainly including industrial flue gas sulfide catalytic removal and resource utilization.

Cu-doped waste-tire carbon as catalysts for the oxidation of sulfamethoxazole

Yuanbo Zhou[1]*
Yang Yu[1]
Qian Ma[1]
Fei Huang[2]
Na Jiang[1]
Xinlu Liu[1]
Yongjun Zhang[1]

[1]School of Environmental Science and Engineering, Nanjing Tech University, Nanjing, 211816, China.
[2]School of Food Science and Pharmaceutical Engineering, Nanjing Normal University, Nanjing, 210023, China.

Abstract

Sulfamethoxazole (SMX) is a typical broad-spectrum antibiotic. Because SMX is widely used in the treatment of infectious diseases, it has been frequently detected in the aquatic environment, which may cause potential ecological risks. However, due to the difficulty in the degradation of SMX and the poor efficiency of traditional treatment methods, it is urgent to develop the degradation technology of SMX. In this study, waste-tire carbon (WTC), as a recycled material, was doped with metal through vibration milling. The Cu-doped WTC exhibited an efficient catalytic activity for the degradation of SMX with H_2O_2 and UV light. The SMX conversion reached 83.85% after 120 min catalytic oxidation under optimal conditions. Besides, to estimate the reactive oxygen species (ROS) concentrations in the Cu-doped WTC/H_2O_2/UV system, a kinetic model with probes was established. Furthermore, scanning electron microscopy (SEM), high-resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS) were carried out to identify the properties of Cu-doped WTC. This work provides a green and efficient catalyst to activate H_2O_2 and an effective protocol to regulate the ratios of ROS in the degradation of organic contaminants with H_2O_2.

Biography:

Yuanbo Zhou is currently pursuing his master's degree in Resources and Environment at the Nanjing Tech University, Nanjing, China. He completed his bachelor's degree in Environmental Science in 2020 from School of Environmental Science and Engineering, Nanjing Tech University, Nanjing, China. He has published two research papers in peer-reviewed journals. Besides, he has one granted Chinese patent. His current research interests include resource utilization of solid waste and the design of carbon-based materials for advanced oxidation processes.

Sludge-ceramic-base monolithic composites via ball milling and 3D printed for levofloxacin removal

Yan Shan[1,2]*
Yifan Yan[1,2]
Jingshan Wang
Han Wu

[1,2,3,4]College of Environmental Science and Engineering, Nanjing Tech University, Nanjing 211816, China

Abstract

In recent years, the pollution of antibiotics to the environment has become more and more serious. The existing activated sludge biological treatment of antibiotic wastewater is far from enough. The treatment effect of advanced oxidation technology is better than other traditional methods, which can degrade antibiotic wastewater very well. As a waste of sewage treatment plant, activated sludge can be reused as a catalyst by carbonization. In this study, activated sludge was used as raw material to print 3D monolithic materials by ball milling with clay and iron-based compounds, so as to realize sludge resource utilization. At same time, the interaction between load of metal, rheological properties and printing properties of composites was studied. In addition, the effect of the ratio of sludge to clay on the degradation of levofloxacin was also investigated. The results show that the 3D activated sludge monolithic material of ball milled iron-based compounds can activate persulfate well, and the continuous degradation of levofloxacin can reach 82 %. The types and functions of free radicals were investigated by EPR test and free radical inhibition test. This work provides an effective strategy for the development of resource sludge utilization to prepare 3D activated sludge monolithic materials and degrade antibiotics in water.

Biography:

Yifan Yan was born in Jiangsu, China, in 1999. He studied at Nanjing Tech University and studied under Professor Xueying Zhang and Associate Professor Shao Yan. His research interests focus on the environment and energy catalysis.

The highly dispersed copper species promoted propane oxidation over Cu-TiO_2 catalyst

Ya Gao
Yarong Fang*

School of Environmental Science and Engineering, Nanjing Tech University, China

Abstract

Volatile organic compounds (VOCs) are important atmospheric pollutants, which not only directly harm human health, but also form the main precursor of tropospheric ozone and photochemical smog. Primary pollutants such as VOCs and nitrogen oxides (NO_x) in the atmosphere, under sunlight, a series of photochemical reactions will occur, generating ozone (O_3), peroxyacetyl nitrate (PAN) and other strong oxidizing secondary pollutants, and then forming photochemical smog, posing a threat to animal and plant health and ecological balance. Short-chain saturated propane (C_3H_8) has high photochemical activity and is one of the top ten major pollutants that promote the formation of tropospheric ozone. Therefore, it is important to develop high efficiency catalysts for catalytic oxidation of VOCs.

We designed and prepared a series of Cu_x-TiO_2 catalyst with different copper loading (x=2.5, 5, 7.5, 10) and evaluate the catalytic performance of propane combustion. The activity evaluation results revealed that $Cu_{2.5}$-TiO_2 oxidation catalyst exhibited best catalytic combustion performance of C_3H_8 (T_{90}=295°C). The results show that the copper species are highly dispersed on TiO_2 surface in $Cu_{2.5}$-TiO_2 catalyst. The theoretical calculation results further confirm the existence of charge transfer (Ti→O→Cu) in the Cu-O-Ti hybrid structure induced from Cu-doped TiO_2, resulting in the lattice distortion of TiO_2 accompany with abundant reactive surface lattice oxygen species. In-situ DRIFTS results show that the surface lattice oxygen O^{2-} can effectively promote the activation and fracture of C-H bond, thus improving the catalytic combustion efficiency of C_3H_8.

Biography:

Ya Gao was born in October 2000 in Heilongjiang Province, China. In 2018, She graduated from Nanjing Tech University with a Bachelor's degree in Resources and Environmental science. She continues to pursue Master's degree in the Nanjing Tech University in 2022. Dr. Yarong Fang is her supervisors of master's degree. Her research interest focus on the development of efficient non-noble based catalysts for degradation of pollutants. She is also attempting to study the DFT calculation for illustrating the catalytic mechanism.

Synthesis and Polymerization of Porphyrin Iron(III) Complexes

Yalan Ning*
Faith Bishop
Tim Bishop

Huston-Tillotson University, USA

Abstract

This project describes how porphyrin-based catalysts can be incorporated in metal-organic frameworks (MOFs) for ring-opening polymerization. It also presents a facile and general method for optimization of the catalytic system by varying the organic struts. After the preliminary trials, the porphyrin-based catalysts may be used as a stereo and chemical selective catalytic reactor, converting a specific monomer out of a mixture of monomers, and into highly tactic polymer. The proposed Metalloporphyrin MOFs could have the benefits of increased catalyst stability and recyclability in contrast to traditional homogeneous ones. And the greatest advantage could come from the high internal surface area of MOFs, enabling advances in the efficiency of catalytic polymerization.

Biography:

Yalan (Christie) is an associate professor at Huston-Tillotson University. She is also the academic advisor and coordinator in the chemistry program. She has also served as a visiting faculty in Air Force and Department of Energy since 2019. She has engaged in research spanning a broad spectrum of areas in inorganic, organic, organometallic, and polymer chemistry, and has developed a strong interdisciplinary background in synthesis.

Preparation of CO2-responsive polymeric nanoparticles

Yeong-Tarng Shieh*

Department of Chemical and Materials Engineering, National University of Kaohsiung, Taiwan

Abstract

Poly(2-dimethylamino) ethyl methacrylate (PDMAEMA) were prepared by the atom transfer radical polymerizations and were investigated as a CO2-triggered emulsifier for emulsion polymerizations of CO2-responsive poly(methyl methacrylate)(PMMA) core-shell nanoparticles in water. PDMAEMA and the synthesized PMMA nanoparticles were characterized by 1H NMR, SEM, particle size, UV-vis, GPC, DSC, and Zeta potentials. The results found that the synthesized PMMA nanoparticles were coated with about 15 wt% PDMAEMA and had diameters of about 125 nm. These core-shell nanoparticles exhibited CO2/N2-responsive dispersion/aggregation behavior in aqueous solutions. The CO2-responsive behavior was associated with the tertiary amine groups of PDMAEMA which was on surface of PMMA nanoparticles. Upon bubbling CO2 in aqueous solution, the tertiary amine groups were protonated resulting in hydrophilic and water-soluble PDMAEMA and thus water-dispersible PMMA nanoparticles. Upon bubbling N2 in aqueous solution, CO2 could be removed and the PMMA nanoparticle dispersion reverted to aggregation. A higher molecular weight of PDMAEMA led to a faster CO2-responsive dispersion but a slower N2-responsive aggregation of the PMMA nanoparticles. This newly developed synthetic system offers a highly efficient route for the fabrication of highly effective stimuli-responsive polymer nanoparticles that enable more precise control over the composition, physical properties, and environmentally responsive performance of nanoparticles in aqueous solution.

Technical Analysis Of Biomass For Potential Application In Energetics

Gursel Abbas[1]*
Rafal Lysowski[2]
Ewelina Ksepko[2]

[1]Hacettepe University, Turkey
[2]Wroclaw University of Science and Technology, Poland

Abstract:

The quest for more sustainable energy sources is driven by the need to reduce greenhouse gas emissions and meet the growing demand for energy. Biomass derived from plants is a promising renewable energy source and could play a significant role in achieving carbon neutrality, especially when burned and combined with effective Carbon Capture and Storage (CCS) technologies. Using agricultural waste or non-recyclable residuals as biofuels is a more environmentally friendly alternative, as it eliminates the need for special biomass cultivation.

This study conducts a technical analysis of biomass obtained from various sources, including wood waste, energy crops, sewage sludge, unused biomass, and different types of algae. The ash content, volatile matter, and total moisture content were determined using ISO standards, and the higher heating value (HHV) was measured using a calorimetric bomb. The results of the analysis were compared with those of brown coal, and the findings indicate a promising potential for biomass as a fuel. The HHV of the samples ranges from 13.1 MJ/kg to 20.7 MJ/kg, with ash content, volatile matter, and total moisture content values similar to those of brown coal.

In addition, the XRD and SEM-EDX analysis of the ash content showed encouraging results for using the ash in cement production due to its high content of Si, Al, Fe, and Ca. The results demonstrate the viability of biomass as a renewable energy source, which could contribute to a more sustainable future.

Biography:

I am currently in my senior year as a chemical engineering bachelor's student at Hacettepe University. Alongside my undergraduate studies, I serve as an undergraduate research assistant in the Chemical Engineering Department. I am the only three-time winner of the Erasmus+ Exchange Program with full scholarshp within the Engineering Faculty of Hacettepe University.

Obtaining Green Energy From Municipal Wastewater Treatment Plants With Environmentally Friendly And Energy-Efficient Technologies

Gursel Abbas*
Ozge Yuksel Orhan

Hacettepe University, Turkey

Abstract:

Waste management is a critical issue, as the growing amounts of domestic and industrial waste are leading to environmental pollution and a threat to public health. Two such waste products, waste sludge and red mud, are of concern due to their negative impact on the environment.

In chemical looping combustion (CLC), five types of sludge from the "Ankara Central Wastewater Treatment Plant" were utilized as fuel, including sewage, excess, raw, anaerobic, and activated sludge. Red mud from "Eti Aluminum" was employed as an oxygen carrier. Analytical methods such as SEM-EDX, XRD, and XRF were used to assess the efficiency of the process, as well as the higher heating value (HHV), moisture content, ash content, and volatile matter analyses.

The results showed that the microscopic shape, morphological structure, and properties of the red mud remained constant after heating to 950 °C, making it suitable for use as an oxygen carrier in CLC with zero CO, N_2O, NO_x, and SO_x emissions. Additionally, the waste sludge was found to be an energy source equivalent to brown coal, and the ash produced could be utilized in cement and fertilizer production due to its high content of Si, Al, Fe, P, Mg, and Ca.

This study represents a significant contribution to the field of waste management, providing a novel technology for the handling of domestic and industrial waste in an environmentally responsible manner. The method offers a zero-waste and zero-carbon footprint approach, helping to mitigate the impact of waste on the environment.

Biography:

I am currently in my senior year as a chemical engineering bachelor's student at Hacettepe University. Alongside my undergraduate studies, I serve as an undergraduate research assistant in the Chemical Engineering Department. I am the only three-time winner of the Erasmus+ Exchange Program with full scholarship within the Engineering Faculty of Hacettepe University.

Construction of Bi(hetero)aryls Mediated by DPZ Photoredox Catalyst

Zuzana Burešová*
Filip Bureš

Institute of Organic Chemistry and Technology, Faculty of Chemical Technology, University of Pardubice, Czech Republic

Abstract

Hundred years ago, G. Ciamician carried out the first photochemical processes and established fundamentals of the current photoredox catalysis.[1] Transformation of solar energy to the energy of a chemical bond is very attractive process, which can be accomplished via photoredox catalysis. A suitable catalyst, either metal-based or organic, play a key role in such photochemical reactions. Dicyanopyrazine (DPZ) photoredox catalyst enables various radical processes[2] including visible light-induced C-C bond formation affording bi(hetero)aryls.[3] We have developed a facile DPZ-catalyzed method to cross-couple five- and six-membered rings such as pyrrole, imidazole, oxazole, thiazole and diazines (pyridine and pyrimidine) with various (hetero)aryl halides. The plausible mechanism involves three reaction pathways - photoredox catalysis, photoinduced disproportionation process, and electron donor-acceptor complex. The developed DPZ-mediated cross-coupling reactions afforded target bi(hetero)aryls in good to excellent yields and photoredox catalysis proved to be an exclusive reaction pathway for less reactive bromo- and chloro-derivatives.

Biography:

Zuzana Burešová studied organic chemistry at the University of Pardubice, where she finished her master and doctoral studies in 2016 and 2019, respectively. In 2018, she pursued internship at the FAU (Erlangen, Germany) under guidance of Prof. M. Kivala. Her current research activities focus mainly on design and synthesis of organic p-systems and visible light-initiated organic transformations via photoredox catalysis.

Alkylidenes from Tungstacyclopentane Complexes via Photoinduced α-H Abstraction or Ring-Contraction

René Riedel*
Richard R. Schrock
Matthew P. Conley
Veronica Carta

University of California, Riverside, CA

Abstract

For over 50 years an outstanding question in organometallic chemistry and catalysis has been how heterogeneous and homogeneous olefin metathesis catalysts that contain Mo, W, or Re are formed from olefins. We recently showed that d2 tungsten styrene complexes can be protonated slowly with dimethyl-anilinium to yield a mixture of styrene and phenethylidene complexes. The intermediate is a cationic phenethyl complex that can be deprotonated either at the α or the β position. A plausible mechanism in the absense of a Brønsted acid involves the formation of metallacyclopentane complexes. While unsubstituted analogs are often proposed as intermediates in the catalytic dimerization of ethylene, they are considered inactive byproducts of metathesis. Therefore, we turn to the question concerning how alkylidenes may be formed in the absence of a Brønsted acid in solution employing the effect of visible light on metathesis–inactive but photoactive square pyramidal d0 tungstacyclopentane complexes. Temperature dependent photolysis studies and preliminary DFT calculations suggest that irradiation at 405 nm promotes an electron from the two W-C s-bonds (HOMO) to the essentially empty dxy orbital (LUMO) to give a W(V) intermediate comprising a butyl radical. While unsubstituted tungsten imido metallacyclopentane derivatives subsequently undergo ring contraction via 1,2-hydrogen atom migration, α-hydrogen abstraction dominates in cases of b,b'-disubstituted analogs such as dimethyl-, dipentyl, or bicyclic tungstacyclopentanes to give corresponding alkylidenes. Those

results further raise the possibility that ambient light might have an effect in some metathesis reactions involving tungsten-based imido alkylidene olefin metathesis catalysts, if not others.

Biography:

René Riedel grew up in Bavaria, Germany, and obtained his M.Sc. in Chemistry from FriedrichAlexander-University Erlangen-Nuremberg. In the course of his PhD project under the supervision of Professor Anthony G M Barrett at Imperial College London, he established several research collaborations focusing his interest on alkali metal solutions and their synthetic applications. Since he joined Professor Richard R Schrock's group at UC Riverside he studies the formation of alkylidene complexes from olefins under the influence of visible light.

Oral Presentations

Fabrication of ZnO Thin Films using Mist Chemical Vapor Deposition and Evaluation of its Photocatalytic Activity

Chaoyang Li

Kochi University of Technology, Japan

Abstract Not Available!!!

Physicochemical and (Photo)Electrochemical Characterization of M-Biox (M=Pd, Cu, Pd-Cu and X = Cl, Br, I) Composites Towards the CO2 Reduction

J. Manuel Mora-Hernandez

CONACYT - Universidad Autónoma de Nuevo León, México

Abstract Not Available!!!

Ab-initio Studies of Elemental Processes in Water Splitting Technologies

Tadashi Ogitsu

Lawrence Livermore National Laboratory, Livermore, CA

Abstract Not Available!!!

Cathodization based Tuning of TiO_2 Nanotube Arrays as (Photo)Electrocatalysts for Environmental and Energy Applications

Kangwoo Cho*
Hyeonjeong Kim
Doyeon Park

Pohang University of Science and Technology, Republic of Korea

Abstract:

The (photo)electrochemical activities of TiO_2 proved to be enhanced by cathodization in mild conditions. A self-doping altered the level of self-dopants (Ti^{3+} and oxygen vacancy) to tune the band structure, to improve light absorbance, electrical conductivity, capacitance, and charge transfer. In this study, TiO_2 nanotube arrays (TNAs) prepared by anodization of Ti foil were systematically underwent variable cathodization conditions, including current density/duration, pH/buffering intensity of electrolyte, sequence of annealing, and existence of external dopant (Nb^{5+}). The self-doping of anatase TNA reduced the band gap to 2.4 eV (blue TNA), while the same sequence for amorphous TNA gave degenerately doped black TNA. The self-dopants (Ti^{3+}) were exclusively located on surface for blue TNA, whereas penetrated into bulk structure for

black TNA with quasi-permanent lattice distortion. The level of passed charge was more effective than the current density. The pH and buffering intensity of electrolyte switched the levels of Ti^{3+}, proton, and oxygen vacancy on surface, which in-turn affected the incident photon-to-current conversion efficiency in 300 - 400 nm range. Upon the optimized self-doping conditions, the black TNAs were suitable for EC applications (direct/mediated water treatment), whereas the blue analogous could be utilized for PC/PEC water treatment with solar energy conversion into H_2. A cathodization-based doping of Nb^{5+} on anatase TNA induced oxygen/cation vacancy to intensify the PEC performance under UVC irradiation. The results of this study would broaden the usage of TiO_2 nanomaterials by engineering the physico-chemical properties depending on variable energy input and application scenarios.

Biography:

Kangwoo Cho is professor in Pohang University of Science and Technology (POSTECH). He received B.S./M.S. in Civil, Urban, and Geosystem Engineering from Seoul National University in Korea and served as a research scientist at Korea Institute of Science and Technology (KIST) from 2006-2017. During 2010-2015, he finished Ph.D degree requirements at California Institute of Technology (Caltech) under the supervision of Prof. Michael R. Hoffmann. Dr. Cho's research interests nowadays span broadly in advanced redox processes based on (photo)electrochemistry, electrochemical intensification of physical/biological water treatment practices, and engineering of electro-catalysis for environmental application.

Visible-Light Mediated Organic Transformations Catalyzed by DicyanoPyraZine

Filip Bureš*
Zuzana Burešová

Institute of Organic Chemistry and Technology, Faculty of Chemical Technology, University of Pardubice, Czech Republic

Abstract:

In recent years, photoredox catalysis evolved into an attractive and industrially important tool of modern organic synthesis. Photoredox catalysts, resembling natural chlorophyll's mechanism of action, enable radical chemical transformations to be carried out at very mild reaction conditions. Upon excitation, these catalysts behave as strong one-electron reductant/oxidant that may be employed in a variety of fundamental and advanced synthetic protocols. Besides well-explored coordination compounds such as $Ru(bpy)_3$ and $Ir(ppy)_3$, organic dyes, such as Eosin Y, Rose Bengal, Flavins, etc., are also employed as catalysts. However, synthetic dyes featuring properties tunable towards the given photoredox process are currently the most burgeoning class of catalysts.[1] In 2014, we have developed purely organic photoredox catalyst based on DicyanoPyraZine (DPZ),[2] which proved to be highly active in visible light-initiated reactions including various C-C bond formations, enantioselective photoreductions, photooxygenations, annulations, etc.[3] Hence, DPZ development and its fundamental properties and applications across photoredox catalysis will be discussed.

Biography:

Filip Bureš finished his master and doctoral studies in organic chemistry at the University of Pardubice in 2002 and 2005. Subsequently, he pursued studies at the LMU (Germany) and postdoctoral fellowship at the ETH Zűrich (Switzerland) under guidance of Prof. P. Knochel and Prof. F. Diederich. After his return to Pardubice, he has been habilitated in 2010 and subsequently awarded a full professor in December 2017. His current scientific interest involves advanced organic and organometallic materials with manifold applications including catalysis.

Electrocatalytic Conversion of CO2 in a Membrane Electrode Assembly Flow Electrolyzer

Siyu Zhong1*
Alexander Navarrete Munoz[1]
Peter Holtappels[1]
Roland Dittmeyer[1]

[1]Institute for Micro Process Engineering (IMVT), Karlsruhe Institute of Technology (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Abstract:

Electrocatalytic carbon dioxide reduction reaction (CO2RR) to chemicals and fuels is a popular candidate for scaling up electrochemical production in the "Power to X" process. H-cell electrolyzers have been widely used to quantify the activity of electrocatalysts; however, slow mass transfer leads to undesirably low current densities.

In this study, the concept of a 0-gap membrane electrode assembly (MEA) flow electrolyzer is extracted to create efficient mass transfer and achieve low impedance. Ti current collectors with circular spiral channels were designed and fabricated, and the depth of the gap was adjusted to accommodate the thickness of several ion exchange membranes and gas diffusion layers, so that the gas tightness and insulation of the reactor were ensured. The reactant CO2 gas and liquid electrolyte flow continuously at the cathode and anode, respectively, while the catalysts sprayed on the gas diffusion layers are in direct contact with the ion exchange membrane. Besides, the reaction kinetics are also enhanced by increasing the temperature when the custom reactor and self-build test bench can operate at conditions up to 20 bar and 180 degrees Celsius.

Here, the effects of temperature, pressure, and flow rate on the conversion of CO2 to hydrocarbons in an MEA electrolyzer are investigated to obtain high current density, product faraday efficiency, and energy efficiency. The optimal operating conditions will be extended to other electrolytic cells in the future.

Biography:

Siyu Zhong received her Master of Science degree in Physics from Hunan University in 2019. She is a Ph.D. candidate in Chemical Engineering under the supervision of Prof. Roland Dittmeyer at Karlsruhe Institute of Technology. Her research interests are in CO2 electrocatalysis and Li/Na-ion batteries, and she has full experience in nanomaterial synthesis, reactor design, test bench construction, and Comsol simulation.

Porphyrin Small Molecules for Photocatalytic Hydrogen Evolution

Xunjin Zhu*
Kailin Zheng
Govardhana Bodedla

Department of Chemistry and Institute of Advanced Materials, Hong Kong Baptist University, Waterloo Road, Kowloon Tong, Hong Kong, P. R. China.

Abstract:

Recently, photocatalytic hydrogen evolution (PHE) has been intensively researched for producing H2 as a clean energy and renewable fuel. In this report, we first reported the naphthalimide (NI) chromophore conjugated Zn(II)-porphyrin as photosensitizer for enhanced the PHE.1 This is mainly because a Förster resonance energy transfer (FRET) from the NI energy donor to the porphyrin ring energy acceptor improves the light-harvesting property and stabilizes the photoexcited singlet states of porphyrin with a longer electron lifetime, and further facilitates an efficient photoinduced hole-electron separation and fast migration in the photocatalytic systems. Next, we further demonstrated that that NI-conjugated Pt(II)-porphyrins are capable of undergoing highly efficient cocatalyst-free PHE due to the FRET and the long-lived triplet excited states of Pt(II)-porphyrin. At the same time, the conjugation of Ir-complex onto Zn(II)-porphyrin through a phenyl linkage, leads to a synergistic effect of aggregation-induced emission (AIE), aggregation caused by quenching (ACQ) inhibition, and FRET.2 As a result, this complex exhibits highly efficient cocatalyst-free PHE because of efficient UV-visible light-harvesting, longer photoexcited electron lifetime, and thereby more efficient electron transfer from the photoexcited porphyrin to the proton for water reduction.

Biography:

Zhu Xunjin is currently Associate Professor at the Department of Chemistry, Hong Kong Baptist University. Dr. Zhu obtained his PhD degree in 2006 at Hong Kong Baptist University, and worked as post-doctoral fellow from 2006 to 2010 at the University of Texas at Austin and Georgia Institute of Technology, next, started his academic career as Research Assistant Professor and Assistant Professor from 2010 to 2019 at the Department of Chemistry, Hong Kong Baptist University. His current research interests focus on the design and synthesis of porphyrin materials for various applications from organic solar cells, artificial photosynthesis, to electrocatalysis.

A new process for water treatment associating photocatalysis and hydrothermal processes

Chantal Guillard*
Insaf Abdouli
Frederic Dappoze
Marion Eternot
Nadine Essayem

University Lyon, University Claude Bernard, CNRS, IRCELYON, France

Abstract:

Photocatalysis is a green catalytic process for removing low concentration of pollutant in water, due to the possibility to activate photocatalyst at ambient temperature and under atmospheric pressure. However, the industrial applications of this advanced oxidation process have been limited due to the low kinetic of this type of process and the byproducts generated which can be more toxic than the initial pollutant. Beside the photocatalytic process, hydrothermal process is an efficient process for water treatment containing high concentration of pollutant. However, this process is energy intensive due to high operating temperatures and the use of high pressures. Moreover, generally, noble metal is used such as Pt, Au, Pd, Ru loaded on different support, Al2O3, TiO2 The objective of our work has been to investigate the efficiency of the combination of these two processes using different nature of TiO2 (rutile, anatase and mixture of anatase/rutile) as catalyst and relatively low temperature and pressure (120°C and 5 Bar). In this regard, the mineralization of a model pollutant and of real effluent such as black liquor

have been performed under pure photocatalysis, pure hydrothermal process and hydrothermal process assisted by photocatalysis. a water treatment this new process by investigating. This new concept of coupling hydrothermal process and photocatalysis have been shown very interesting for water treatment by favoring the mineralization of carbon. A discussion of mechanism is proposed considering the important impact of the nature of TiO2.

Biography:

I am Doctoc-ès-Sciencesin Catalysis and have been working in Photocatalysis at the CNRS since 1989. Now I am CNRS Director at Ircelyon, Lyon university. I am the authors of 203 papers, 281 communications and 8 patents center on Photocatalysis. My H-factor is 56. My studies are devoted to basic research to better understand the efficiency and mechanisms of photocatalysis in water and air treatment, energy production and biomass valorization. I also coupled photocatalysis with other processes, developed new photocatalytic materials in particular photocatalytic optical fiber fabrics and worked with microbiologists to improve the knowledge on the inactivation of microorganisms

Oxo-Metal Catalyzed Deoxydehydration Reactions

Alex John1*
Nathan J Wagner
Fernando J. Alfaro
Paul Lam
Haruka Takenaka
Ying Wang
Paula M. Magat
Eunice C. Castro
Emily Corona
Paul W. Musharbash
Jerome B. Torres

California State Polytechnic University, Pomona, CA, USA

Abstract:

Development of practical methods for deoxygenation of biomass is crucial for reducing the current global dependence on fossil resources. The deoxydehydration reaction which converts vicinal diols to olefins is particularly unique in this respect given the highly oxygenated nature of biomassderived. Established methods for effecting this reaction rely on catalysts based on rhenium, a precious metal. Catalytic methods based on earth-abundant metals such as molybdenum and vanadium are less explored, and known methods are plagued by the need for high catalyst loadings,high reaction temperatures as well as low reactivity. We have explored the use of oxo-molybdenum catalysts supported over ancillary ligands in effecting the deoxydehydration reaction. Catalytic activity (10 mol % catalyst, 170 ?C, 2-24 hours) was evaluated as a function of steric and electronic variations on the ligand backbone to establish structure–activity correlations. Olefin yields as high as 99 % were achieved using the bio-based diol substrate, diethyl tartrate. The ligand backbone and the nature of the donor arm were found to be critical in dictating catalytic activity.

Biography:

Alex John is an Associate Professor of Organic Chemistry at California State Polytechnic University Pomona. Prior to this he did post-doctoral research at the University of Oklahoma (Advisor: Prof. Kenneth M Nicholas) and as part of the Center for Sustainable Polymers at the University of Minnesota (Advisors: Prof. William B Tolman & Prof. Marc A Hillmyer). His research interests are in sustainable chemistry with a focus on developing catalytic methods for converting biomass-derived molecules into platform chemicals, green oxidation reactions, and polymers from renewable molecules

Pilot scale solar photocatalysis for treatment of polluted air and water: Croatian case study

Ivana Grčić*[,1]
Lucija Radetić[1]
Ivana Presečki[1]
Marija Tomaš[1]
Paula Benjak[1]
Ivan Brnardić[2]

[1] University of Zagreb, Faculty of Geotechnical Engineering, Hallerova aleja 7, 42000 Varazdin Croatia
[2] University of Zagreb, Faculty of Metallurgy, Aleja narodnih heroja 3, 44000 Sisak, Croatia

Abstract:

Over the several last decades, solar photocatalysis has been proven as a viable option for removal of emerging and priority pollutants from the environment. Widespread research has been made into the photocatalytic properties of TiO_2 because of its ability to break down and destroy many types of pollutants. According to relevant patent databases and recent publications, a variety of reactors have been proposed for both air and water treatment. The compound parabolic collector (CPC) reactor represents an optimal reactor and is recognized as state-of-the-art from the aspect of reactor geometry and incident irradiation usage. A reactor system can be easily scaled-up and installed at the outlet of municipal water treatment plants and industrial wastewaters or be used as an emerging system for water purification on terrain sites. Since the CPC reactor represents a continuous system, its applicability was assumed for air treatment as well.

In this work, we demonstrate solar photocatalysis in the CPC reactor using TiO_2-based photocatalysts supported on a glass fiber mesh. The degradation extents and tentative pathways of several typical micropollutants in surface waters (e.g. ibuprofen, carbamazepine and others) whose presence has been confirmed using non-target analysis using the LC-MS/Q-TOF system are shown. The purification of air polluted by NOx and ammonia was performed to demonstrate the applicability of the CPC reactor for active air pollution control. In addition to the CPC reactor, a specially designed photocatalytic wind tunnel was used to estimate the extent of airborne pollutants degradation by solar photocatalysis in a simulated environment.

Biography:

Ivana Grčić works as an associate professor at the University of Zagreb. Her research interests focus on water and air purification, ultrasound, photocatalysis and respective modeling. Other

relevant areas of her research include the reuse of waste materials for photocatalysis and the preparation of catalysts. She had training at University of Nottingham, UK, regarding the comprehensive modeling of the photocatalytic oxidation process. She is a leader and coordinator of projects funded by the European Regional and Development Fund focused on the development of viable technology for air and water treatment based on solar photocatalysis.

Z-Scheme Heterojunction Consisted by rGO/CeO2/TiO2 for Photothermo-Catalytic Oxidation of Elemental Mercury

Ji-Ren Zheng1*
Chung-Shin Yuan

Institute of Environmental Engineering, National Sun Yat-sen University, Taiwan, ROC

Abstract:

This study explored the photothermo-catalytic oxidation of Hg0 using Z-scheme heterojunction rGO/CeO2/TiO2 at 100-200℃. The surface properties of the photothermocatalysts were initially measured. An annular tubular photocatalytic reaction system was self-designed to conduct the Hg0 oxidation experiments. SEM and HR-TEM images showed that the modification of rGO could make the nanoparticles evenly distributed on the surface of rGO thus increasing the specific surface area. XRD results showed that the crystallization of TiO2 was mainly in anatase and graphene oxides were successfully reduced. XPS results showed that Cerium presented mainly in Ce(III), the oxygen vacancies of Ce(III) could efficiently capture the oxygen in the atmosphere. The oxidation efficiency of Hg0 with reaction temperature was in the order of η100℃ > η150℃ > η200℃. Modification of rGO to CeO2/TiO2 could significantly enhance the oxidation efficiency of Hg0 at high temperature. In the atmosphere of N2+Hg0+NO, low NO concentrations (300 ppm) enhanced the oxidation efficiency of Hg0 . In the atmosphere of N2+Hg0+SO2, SO2 competed with Hg0 for the active sites on the surface of photothermocatalysts and inhibited the oxidation of Hg0 , however, the modification of rGO could concur the adsorption competition effect maintaining high oxidation efficiency. XPS results found that SO2 and NO were oxidized to sulfate and nitrate, respectively, and deposited on the surface of the photothermocatalysts. EPR results further confirmed the existence of Z-scheme heterojunction and the active radicals produced by rGO/CeO2/TiO2.

Biography:

Ji-Ren Zheng is a doctoral student in the Institute of Environmental Engineering at National Sun Yat-sen University under the supervision of Distinguished Professor Chung-Shin Yuan. His research interests include the preparation of catalysts, and photocatalytic oxidation of air pollutants, especially the elemental mercury emitted from coal-fired power plants.

Polymeric Nanoparticle Catalysts with Enzyme-Like Catalytic Efficiency and Selectivity for Glycan and Ester Hydrolysis

Yan Zhao*

Department of Chemistry, Iowa State University, Ames, IA 50014, USA

Abstract:

Although chemists rightfully argue that enzymes are “not different, just better” than synthetic catalysts, artificial enzymes created on purely synthetic or semi-natural platforms generally do not match their natural counterparts in performance. The deficiency of artificial enzymes

has many reasons but a main roadblock is the lack of suitable synthetic strategies to construct multifunctional active sites with accurately positioned binding and catalytic groups. We present methods to convert dynamic micelles into cross-linked polymeric nanoparticles with well-defined binding sites through molecular imprinting. The nanoconfinement of the polymerization and cross-linking yield an extraordinary templating effect, with the imprint/nonimprint ratio in binding frequently reaching hundreds and sometimes 10,000. Installation of catalytic groups through postmodification turns the water-soluble nanoparticles into enzyme-like catalysts, with biomimetic or unnatural catalytic motifs. Our synthetic cellulases outperform some natural enzymes in cellobiose hydrolysis, with a k_{cat}/k_{uncat} value up to 10^{10}. Our synthetic esterase could hydrolyze nonactivated alkyl esters at room temperature and neutral pH, while more reactive aryl esters stay intact in the same solution. As robust cross-linked polymeric nanoparticles, these "artificial enzymes" can function under conditions totally impossible for biocatalysts and can be converted into recyclable heterogenous catalysts when clicked onto a solid support.

Biography:

Yan Zhao received his B.S. in chemistry from Lanzhou University in 1992 and Ph.D. from Northwestern University in 1996. After a postdoctoral stay at the University of Illinois, he worked for the Procter & Gamble Company from 1998 to 2002 and is currently a professor of chemistry at Iowa State University. His areas of interest include design and synthesis of biomimetic molecules, polymers, and nanomaterials and using them as synthetic receptors, artificial enzymes, molecular transporters, and sensors for chemical and biological applications.

Synthesis and characterization of silver integrated MXene and reduced Graphene oxide nanocomposites for photocatalytic degradation of dye DB-24

Kishore Chand [a*]
Yujin Chen [a*]
Hemant J. Sagar [b]

[a] Key Laboratory of In-Fiber Integrated Optics, College of Physics and Optoelectronic Engineering, Harbin Engineering University, Harbin 150001, China.

[b] Institute of Ship Technology (ISMT), University of Duisburg-Essen, 47057, Duisburg, Germany.

Abstract:

The discovery of 2D materials extended the pool of nanomaterials for wide range of applications. High conductivity, catalytic efficiency and hydrophobicity led to growing research interest for water treatment applications. In this work, two types of nanocomposites were prepared using heretofore methods practiced already and widely reported in literature. Nanocomposites based on Graphene oxide (GO) was produced by modified Hummer's method and MXene (MAX), by etching the MAX phase into hydrogen fluoride solution (selectively etching method). A new type of nanocomposites, reduced Graphene Oxide-Silver nanoparticles (rGO-Ag) and. MXene-silver nanoparticles (MAX-Ag) were synthesized from the respective pristine materials (GO and MAX). The resultant products were characterized successfully using advanced tools and it was found that adjunct Ag particles integrated on the parent nano films forming a secondary phase of increased electro-catalytic functionality. The products were found to have drastic improvement in catalytic degradation reaction in simulated wastewater. For confirmation, reduction reaction of Direct Blue-24 dye was executed for known concentration of nanocomposites. It was acquired that MAX-Ag showed superior catalytic activity compared to rGO-Ag nanocomposite films. The results from this research may find a useful application for textile wastewater management and other industrial sectors using mutagenic and carcinogenic chemicals having azo and/or phthalocyanine groups in their structure.

Keywords: MXene; MXene-Silver nanocomposite, reduced Graphene Oxide-Silver nanocomposite; nano particles; nano-catalyst

Biography:

Kishore Chand is a research scholar at the Harbin Engineering University, China. His research focuses on the synthesis of metal nanoparticles, graphene, MXenes and their nanocomposites for photocatalyst dye degradation, as well as anion exchange membrane water electrolysis. In 2013, he received his master's degree (M.E) from the MUET, Pakistan. As a first author, he published more than five research articles.

Synthesis of Multi-metallic Nanocatalysts Using a Dendrimer Reactor

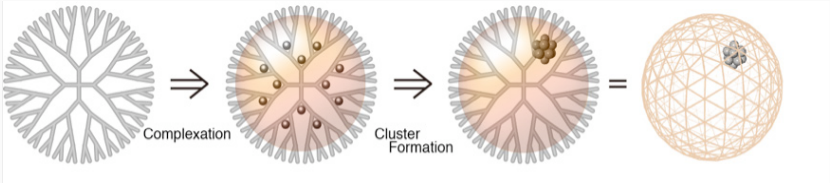
Kimihisa Yamamoto

Tokyo Institute of Technology, 4259 Nagatsuta, Yokohama 226-8503, Japan

Abstract:

Dendrimers are highly branched organic macromolecules with successive layers or "generations" of branch units surrounding a central core. Organic inorganic hybrid versions have also been produced, by trapping metal ions or metal clusters within the voids of the dendrimers. Their unusual, tree-like topology endows these nanometer-sized macromolecules with a gradient in branch density from the interior to the exterior, which can be exploited to direct the transfer of charge and energy from the dendrimer periphery to its core.

We show that $AuCl_3$, $SnCl_2$, $FeCl_3$, and so on complexes to the imines groups of a spherical polyphenylazomethine dendrimer in a stepwise fashion according to an electron gradient, with complexation in a more peripheral generation proceeding only after complexation in generations closer to the core has been completed. By attaching an electron-withdrawing group to the dendrimer core, we are able to change the complexation pattern, so that the core imines are complexed last. By further extending this strategy, it should be possible to control the number and location of metal ions incorporated into dendrimer structures, which might and uses as tailored catalysts, building blocks, or fine-controlled clusters for advanced materials. The metal-assembly in a discrete dendrimer molecule can be converted to a size-regulated metal particle with a size smaller than 1 nm as a molecular reactor(Fig.). Due to the well-defined number of metal clusters in the subnanometer region, its property is much different from that of bulk or general metal nanoparticles. The chemistry of nanocatalysts on the sub-nanometer scale is not yet well understood because precise multi-metallic nanoparticles are difficult to synthesize with control over size and composition. The template synthesis of multi-metallic sub-nanocalaysts is achieved using a phenylazomethine dendrimer as a macromolecular template.



Palladium nanoparticles encaged within amine-functionalized metal-organic frameworks: Extremely efficient multifunctional catalysts for base-free hydrogenation of various aldehydes and ketones.

Abu Taher[1, 2*]
Shohel Ahamed[1]
Ik-Mo Lee[2]

1 Department of Industrial and Production Engineering, European University of Bangladesh, Mirpur, Dhaka-1216, Bangladesh
2Department of Chemistry, Inha University, Incheon 402-751, South Korea.

Abstract:

A palladium nanoparticle (Pd NP) containing metal organic framework (MOF) is described as an extremely efficient multifunctional catalyst for hydrogenation of various aldehydes and ketones in 2- propanol. The catalytic efficiency was demonstrated by the high conversion of the diverse aldehydes and ketones with 100 % selectivity under mild reaction conditions that readily afford quantitative yields (up to 98 %). The size, shape and morphology of the as-prepared catalyst were well-preserved after respective recycling cycles and the catalyst could be reused several times without treatment. Importantly, the simple recovery and excellent selectivity of the as-prepared catalyst for hydrogenation are noteworthy advantages of the present catalytic method. More importantly, this research has showed the remarkable benefits of MOF-based Pd NP as multifunctional catalyst, while the reaction proceeded smoothly at room temperature to give corresponding product without any external base or other additives.

Production of Composite PAN-Fibers Functionalized with Nanoscale NiO Catalysts For Enhanced Gas Sensing Properties

Imash Aigerim

Institute of Combustion Problems, Kazakhstan

Abstact Not Available!!!

Chemo-Enzymatic Synthesis of Pure Enantiomers of β-Antagonists Bisoprolol and Betaxolol

Elisabeth Egholm Jacobsen*
Lucas Boquin
Susanne Hansen Troøyen

Department of chemistry, Norwegian University of Science and Technology, Høgskoleringen 5, 7491 Trondheim, Norway

Abstract:

β-Blockers are one of the classes of drugs which plays a relevant role in the treatment of various human diseases such as hypertension, angina pectoris, migraines and tremors. β-Blockers are βadrenergic antagonists, which affects the β-adrenergic receptors found in a variety of places in the human body, with most efficiency in the heart and vascular system [1]. Only a few β-blockers are manufactured with the single enantiomer Active pharmaceutical ingredient

(API), even though for most β-blockers the (S)-enantiomers are the more potent enantiomer [2]. Several negative side effects from the "wrong" enantiomer are also known. Due to this there is a need for effective and green methods for production of single enantiomers of these widely used drugs. We have for some time studied the synthesis mechanisms for production of single enantiomers of several β-blockers [3-5]. Here we present our results of producing the pure enantiomers of (S)-bisoprolol and (S)- betaxolol (Figure 1)[6-8].

Biography:

Elisabeth Egholm Jacobsen completed her MSc degree in Organic chemistry and Biotechnology at the Norwegian University of Science and Technology, Department of Chemistry in 1999 after employment as an analytical chemist in the cosmetic industry for 11 years. She earned her PhD in Organic Chemistry in 2004. Since 2005 she helds an associate professor position at the same department. Her research focusses on synthesis of enantiopure biologically active compounds, f. inst. enantiopure drugs, by use of enzymes as chiral catalysts. Her teaching has been focusing on green chemistry, biocatalysis, general and organic chemistry, natural product chemistry, spectroscopic methods and chromatography.

Insights into the Catalytic Mechanism of Nitrile Hydratases

Richard C. Holz[1,2*]
Callie Miller[1]
Irene Ogutu[1,2]
K.P. Wasantha Lankathilaka[1,2]
Natalie Gumataotao[4]
Brian Bennett[3]
Adam Fiedler[2]
Dali Lui[4]

[1]Contribution from the 1Department of Chemistry, Colorado School of Mines, Golden, Colorado 80401
[2]Department of Chemistry, Marquette University, P.O. Box 1881 Milwaukee, Wisconsin 53201
[3]Department of Physics, 540 N. 15th St., Marquette University, Milwaukee, Wisconsin 53233
[4]Department of Chemistry and Biochemistry, Loyola University, Chicago, Illinois 60660.

Abstract:

Nitrile hydratases (NHases, EC 4.2.1.84) are exceptional biocatalysts with broad substrate specificity but strict stereoselectivity, that are capable of hydrolyzing nitriles under mild reaction conditions. As such, they are in high demand as biocatalysts in preparative organic and pharmaceutical chemistry applications, as nitriles represent an important synthon that adds an extra carbon atom to an alkyl chain. NHases have been exploited in several industrial applications, most notably in the production of acrylamide, adiponitrile, and nicotinamide. NHases have also been employed in the bioremediation of chemical and wastewater runoff, specifically for the hydration of nitrile-based pesticides such as bromoxynil. NHases are α2β2 heterotetrameric holoenzymes. The α-subunit includes a highly conserved amino acid sequence (CXYCSCX) that forms the metal binding site. NHases contain either low-spin (S = 1/2) Fe(III) ('Fe-type') or low-spin (S = 0) Co(III) ('Co-type') in their active sites. X-ray crystallographic studies on both Fe-type and Co-type NHases reveal identical active sites, containing a six-coordinate metal ion bound by three cysteine residues, two amide nitrogens, and a water or hydroxyl moiety (Figure 1). Two of the active site cysteine residues are post-translationally modified to cysteine-sulfinic acid (–SO2H) and cysteine-sulfenic acid (–SOH), respectively. We recently proposed a catalytic

mechanism with a hitherto unknown role for a sulfenic acid (αCys-OH) ligand as an active site nucleophile, which was subsequently corroborated by time-resolved X-ray crystallography and DFT. This catalytic mechanism will be discussed including new information on potential catalytic intermediate steps.

Biography:

Rick Holz is currently the Provost and a Professor of Chemistry at the Colorado School of Mines and is a member of the Quantitative Biological Engineering faculty. He was inducted into the University of Minnesota Duluth Academy of Science and Engineering, Figure 1. NHase active site (PDB:1IRE) is an Associate Editor of the journal Frontiers in Chemical Biology, and is on the editorial board of the journal Catalysts. He is member of the American Chemical Society, the Society of Biological Inorganic Chemistry, and the American Society for Biochemistry and Molecular Biology. He is the author of more than 120 scientific papers in the fields of inorganic, bioinorganic, and biophysical chemistry.

Reliable Modeling of Homogeneous 3d-Transition Metal Electrocatalysis

Andreas Hansen[1]*
Hagen Neugebauer[1]
James Shee[2]
Demyan E. Prokopchuk[3]
Stefan Grimme[1]

[1]RFWU Bonn, Mulliken Center for Theoretical Chemistry, Germany
[2]UC Berkeley, Department of Chemistry, USA
[3]Rutgers University-Newark, Department of Chemistry, USA

Abstract:

Homogeneous 3d-transition metal electrocatalysis is a promising approach, e.g., for sustainable fuel production through H_2 generation or CO_2 reduction with earth-abundant metals. Computational chemistry can make an important contribution to the development of more efficient catalysts, e.g., by elucidating the underlying mechanisms or tuning the ligands to achieve lower overpotentials, higher turnover frequencies, and better substrate selectivity. However, it is challenging to find robust quantum chemical methods that can be reliably applied to the size of the target system (30-150 atoms) and the often quite complicated electronic structure of typical electrocatalysts. Using a newly assembled benchmark set of vertical ionization potentials (IPs) comprising 28 moderately diverse 3d TM complexes of practical importance as electrocatalysts (3dTMV), we discuss which diagnostic tools are most informative with respect to a multireference electronic structure and how reliable theoretical reference values for various degrees of static correlation can be generated using sophisticated coupled cluster (CC) and quantum Monte Carlo (QMC) methods. In practical applications, Kohn-Sham density functional theory (KS-DFT), which is the workhorse of catalytic mechanism modeling due to its favorable cost-accuracy ratio, is the method of choice. To provide recommendations to (computational) chemists, we present a thorough evaluation of current and state-of-the-art KS-DFT, including efficient composite methods and special DFT approaches for handling static correlation. We exemplify how electrocatalysts can be reliably modeled with (mostly) KS-DFT-based, multilevel workflows to create synergy with experimental efforts to develop more efficient systems. We also provide an outlook on future challenges, e.g., how to obtain a more accurate description of solvation effects.

Biography:

Andreas Hansen received his PhD in 2012 on the development of local open-shell correlation methods under the supervision of Frank Neese. Since then, he manages, teaches, and researches as academic chief counselor at the Mulliken Center of Theoretical Chemistry of the University of Bonn, Germany, in collaboration with Stefan Grimme. His research focuses on developing quantum chemical methods and workflows, with special focus on compiling comprehensive benchmark sets and protocols for the reliable calculation of reference values for diverse chemical properties.

Pd@Pt Nanodendrites as Peroxidase Nanomimics for Ultra-sensitive ELISA of Cytokines towards Personalized Immunotherapy

Pengyu Chen*

Materials Engineering, Department of Mechanical Engineering, Auburn University, Auburn, Alabama 36849, United States

Abstract:

Simple and sensitive detection of cytokines in biological samples is crucial because of their important roles as cell signaling molecules and disease biomarkers in biomedical science. Colorimetric enzyme-linked immunosorbent assay (ELISA) has been widely recognized as the gold-standard method for the detection of cytokines for decades. However, it remains a challenge to further improve its detection sensitivity as limited by the catalytic activity of enzymes. Herein, we report an enhanced colorimetric ELISA for ultrasensitive detection of interleukin-6 (IL-6, as a model cytokine for demonstration) using Pd@Pt core@shell nanodendrites (Pd@Pt NDs) as peroxidase nanomimics (named "Pd@Pt ND ELISA"), pushing the sensitivity up to femtomolar level. This detection limit was 21-fold lower than that of conventional HRP-based ELISA. The reproducibility and specificity of the Pd@Pt ND ELISA were excellent. More significantly, the Pd@Pt ND ELISA was validated for the analysis of human serum samples with high accuracy and reliability through recovery tests. Our results demonstrate that the colorimetric Pd@Pt ND ELISA is a promising biosensing tool for ultrasensitive determination of cytokines and thus is expected to be applied in a variety of clinical diagnoses and fundamental biomedical studies.

Biography:

Pengyu Chen is currently Hugh and Leoda Francis Endowed Associate Professor in Materials Engineering at Auburn University. He received his B.S. in Materials Science and Engineering from Nanjing University in 2006 and obtained Ph.D. in nanomaterials and biophysics (2012) from Clemson University. He then worked as a research fellow in Mechanical Engineering at the University of Michigan and join Auburn in 2016. He was the recipients of Ginn Faculty Achievement Fellow, NIH Maximizing Investigators' Research Award and NSF CAREER Award. Chen's research focuses on advanced nanomaterial based biosensors for biomarker detection, single cell secretion imaging, and cellular communication.

Biocatalysis by Immobilized Enzymes

Ming-Qun Xu*
Aihua Zhang

Bo Yan
Yi Fang
Guillermo Garcia Marquina
Amogh Changavi
Zhiyi Sun

New England Biolabs, Inc., United States

Abstract:

Immobilized enzymes offer a variety of advantages over free enzymes in solution, including an rapid separation of enzymes and products, circumvention of heat treatment and purification chromatography, and enzyme re-use. Enzyme immobilization, however, can introduce conformational change, spatial confinement, and limited substrate accessibility, resulting in partial or total loss of enzymatic activity. We have engineered covalent and site-specific immobilization of DNA and RNA modifying enzymes and chemical modification of solid support materials, aiming at production of highly active immobilized enzymes with low leaching and high stability. We have successfully applied these immobilized enzymes to library preparations for high throughput DNA and RNA sequencing platforms. We demonstrate that our enzyme immobilization technology enables highly efficient catalysis and robust workflows for research and commercial applications.

Characterization of doped carbon thin films prepared by PVD process as electrode material in electrochemistry

Frank Kaulfuss[1]*
Julius Hebenstreit[1]
Federico Faglia[1]
Cory Rusinek[2]
Volker Weihnacht[1]

[1]Fraunhofer IWS - Institute for Material and Beam Technology, Dresden, Germany
[2]Department of Chemistry and Biochemistry - University of Nevada, Las Vegas

Abstract:

The Laser-Arc process is a PVD technique to synthesize hydrogen-free tetrahedral amorphous carbon (ta-C). The advantage of the process is the formation of an ionized, highly energetic carbon plasma, which forms ta-C coatings on almost all substrate materials without any heating. However, depending on deposition conditions, the sp3-content can be varied over wide ranges and also graphite-like amorphous carbon (a-C) can be deposited by the Laser-Arc process. The (t)a-C coatings are chemically inert and their electrical conductivity depends on the sp3-content and the nanostructure in the coating. Graphite-like a-C-coatings show high potential on stainless steel bipolar plates of fuel cells due to the unique combination of inertness and electrical conductivity.

When (t)a-C is doped with nitrogen (N) and/or boron (B), it exhibits semi-conductor behavior with simi-lar electrical properties to boron-doped diamond (BDD) and glassy carbon (GC) electrodes. In this work, the electrochemical properties of ta-C:B, ta-C:N and ta-C:B:N were studied using common 1-electron transfer redox couples of ferri/ferrocyanide (Fe(CN)6–4/–3) and ruthenium hexamine (Ru(NH3)6+3/+2). Voltammetry and coulometry were used to obtain fundamental redox properties and these values were compared between the different types of ta-C. The potential windows were determined to be > 3.4 V, and in 1.0 M KCl the ta-C:B:N layer remained unaffected even at -3.5 V to 4 V. Several other evaluation metrics were used – stability under anodic and cathodic conditions, corrosion resistance, bioanalyte detection, and others.

Overall, this work furthers the development of advanced carbon electrodes for a variety of electrochemical applications.

Biography:

Frank Kaulfuss studied materials science at the Dresden University of Technology, Germany. During his subsequent work at the Fraunhofer Institute for Material and Beam Technology (IWS), he conducted research on the topic of nanostructured hard coatings and received his Ph.D. in this field in 2018. Since 2017, he is the head of the group Carbon coating technology at the Fraunhofer IWS.

CVD-prepared Supported Fe-oxide Nanoparticle Catalysts for Efficient Air Purification

Byeong Jun Cha*
Young Dok Kim

Department of Chemistry, Sungkyunkwan University, Republic of Korea

Abstract:

A simple temperature regulated-chemical vapor deposition (tr-CVD) method was used to prepare high-performing catalytic Fe-oxide nanoparticles dispersed on porous supports. Valuable applications of the supported Fe-oxide nanoparticles are introduced, which could overcome the challenges that the current air purification technologies have. Atomic or molecular level understanding about the structures of the catalysts and their relationship with catalytic activity and surface reaction mechanism is also provided.

In the first topic, Al_2O_3 supported Fe-oxide nanoparticles were used as a catalyst for low temperature CO and NO removal, and how the metal-support interaction could govern the catalytic activity is addressed. In the second topic, Al_2O_3 supported Fe-oxide nanoparticles were used as efficient catalytic adsorbent for H_2S, and *in-situ* mechanistic studies on H_2S decomposition under realistic conditions are presented. In the last topic, Fe-oxide nanoparticles were used to promote low temperature activity of commercial Pt nanoparticle catalyst, and related interesting interfacial chemistry of Fe and Pt is studied.

Biography:

Byeong Jun Cha, Ph.D candidate in the chemistry department of Sungkyunkwan University, grew up in South Korea and received his Bachelor and Master degree in chemistry from Sungkyunkwan University under the supervision of professor Young Dok Kim. He continued his academic study in the same group as a Ph.D student. His doctoral research has been focused on 1) preparation of high-performing and cost-effective nanoparticle catalysts and 2) fundamental surface studies on atomic or molecular level using various *ex-/in-situ* surface analyzing tools. He recently finished his dissertation defense, and is looking forward to continuing his research as a post-doc researcher.

The next generation of food colorants derived from nature: Efficient production of pyranoanthocyanins.

Gonzalo Miyagusuku-Cruzado*

Danielle M. Voss
M. Monica Giusti

Department of Food Science and Technology, The Ohio State, Columbus, Ohio, USA

Abstract:

Consumer demand and clean label trends are driving the food industry to find alternatives to artificial food colorants. Pyranoanthocyanins are anthocyanin-derived pigments with vivid colors and improved stability, making them promising alternatives. However, their scarcity in nature and slow formation in food hampers their viable application. Previous studies have shown that pyranoanthocyanins can be formed in model wine systems using hydroxycinnamic acids as cofactors. However, we hypothesized that pyranoanthocyanin formation could be improved by selecting for anthocyanin sources and more reactive cofactors. In our preliminary study we found that copigmentation with ferulic acid increased the chroma half-lives of solutions colored with anthocyanins but reduced monomeric anthocyanin stability. This was later explained by the formation of pyranoanthocyanins. We then hypothesized that this formation could be accelerated by selecting for anthocyanins and cofactors based on their chemical structure. Our study showed that the best anthocyanin-cofactor combination was malvidin-glycosides and caffeic acid yielding almost twice as many pyranoanthocyanins as the second most efficient combination. Pyranoanthocyanin synthesis using hydroxycinnamic acids as cofactors includes a decarboxylation step. We hypothesized that 4-vinylphenols, decarboxylated hydroxycinnamic acids, could be more efficient cofactors for pyranoanthocyanin production. Our results showed that pyranoanthocyanin production with 4-vinylphenols was faster with higher yields and required less cofactor than with hydroxycinnamic acids. This provides a novel approach for the viable production of these promising, naturally sourced colorants for industrial applications. Future studies will focus on the use of bioreactor level fermentation for the production of pyranoanthocyanins using pigment-rich food byproducts and lactic acid bacteria.

Biography:

Gonzalo Miyagusuku-Cruzado is a Postdoctoral Scholar and Research Laboratory Manager at the Department of Food Science and Technology at The Ohio State University. He received a PhD in Food Science and Technology from The Ohio State University working under the guidance of Dr. Monica Giusti, a master's degree in Bioscience and Biotechnology from Kyushu University in Japan, and a bachelor's degree in Food Engineering from Universidad Nacional Agraria La Molina in Peru. His current research focuses on the study of anthocyanins and anthocyanin-derived pigments and on their more efficient production from food waste and lactic acid bacteria.

Distal Regulation in (Stereo)Selective Catalysis

Anton Vidal-Ferran[1,2]*

[1]Catalan Institution for Research and Advanced Studies (ICREA)
[2]Barcelona; Department of Inorganic and Organic Chemistry, University of Barcelona (UB)

Abstract:

Our research interests encompass the design of efficient (stereo)selective catalysts for transformations of interest, involving the functionalization of alkenes and aromatic compounds. Crucial aspects of this work include modular design of the catalysts; use of versatile synthetic procedures (organic and inorganic transformations, as well as supramolecular processes); incorporation of distal regulation mechanisms for the geometry of the active-site in the transition metal-based

catalytic systems; and kinetic and computational studies of the catalytic cycles (through collaborations). The application of our supramolecular catalytic systems in hydroformylations[a] or other transformations will be discussed.[b]

Biography:

Anton Vidal graduated in Chemistry in 1987 and completed his PhD on the synthesis of heterocycles at IQS (Barcelona, 1992). Throughout two post-doctoral appointments (University Cambridge-Prof. Sanders and University Barcelona-1995-1999) he studied topical areas of chemistry (Supramolecular Chemistry and Enantioselective Catalysis). He complemented his background with industrial experience at Bayer-AG (Leverkusen 2001 – 2003). Following the appointment as Research Professor from ICREA, he started his independent research activities at ICIQ (September 2003). In October 2019, he moved to the Section of Inorganic Chemistry of the University of Barcelona to carry on with his research career.

Is this the Alternative to the Rate-Determining Step in Complex Heterogeneous Catalytic Reactions?

Mirosław Szukiewicz *
Elżbieta Chmiel-Szukiewicz
Adrian Szałek

Rzeszów University of Technology, Faculty of Chemistry, al. Powstańców Warszawy 6, 35-959 Rzeszów, Poland

Abstract:

The kinetics of heterogeneous catalytic reactions is of theoretical and practical importance. Theoretical aspects are concerned with determination of the process run, stages, limitations, etc., while in practical applications kinetic experiments were applied to assist reactor design and scaling up of various processes. Both directions overlap, and in many articles they are discussed simultaneously. The most often applied method is to find a single step that has the strongest influence on the reaction rate. This step is selected from a sequence of elementary steps. In the literature, many works present successful applications of the concept; however, in many instances attempts have failed, e.g., for a relatively simple catalytic process, hydrogenation of propene. In this work, we propose a new mechanism scheme and present a procedure based on graph theory to obtain a precise kinetic equation for the real-world process. The method differs substantially from the rate-determining step approach. On the basis of the catalytic cycle, the general form of the kinetic equation is derived without any additional assumptions. It allows consideration of all possible interactions between the reagents and the species. Statistical analysis provides strong evidence for the correctness of the proposed mechanism. The proposed mechanism and the form of the kinetic equation have not previously been reported in the literature and cannot be derived on the basis of rate-determining step approaches.

Biography:

Szukiewicz studied Chemical Engineering at the Rzeszow University of Technology (RUT), Poland and graduated as MS in 1986. He then joined the research group of Prof. Petrus at the Department of Chemical and Process Engineering, RUT. He received his Ph.D. degree in 1995 at Cracow University of Technology. Furthermore, he obtained DSc (Habilitation) from Łódź University of Technology in Chemical Engineering in 2009. Since 2009 he has worked as a professor in the Department of Chemical and Process Engineering (RUT). His main research interests are chemical reactor engineering and mathematical methods in chemical engineering.

Effect of Zr in Fe-based bimetallic oxide for long chain hydrocarbon synthesis during CO2 hydrogenation

Muhammad Kashif Khan[1,2*]
Sheraz Ahmed[3]
Muhammad Irshad[2]
Yoon Woonjong[3]
Jaehoon Kim[1,2,3*]

[1]School of Chemical Engineering
[2]School of Mechanical Engineering
[3]SKKU Advanced Institute of Nano Technology, Sungkyunkwan University, 2066, Seobu-Ro, Jangan-Gu, Suwon, GyeonggiDo, 16419 (South Korea)

Abstract:

Liquid hydrocarbons such as olefins and paraffins are indispensable chemicals that are used widely as transportation fuels and as feedstocks to synthesize numerous commodity chemicals. Carbon dioxide can be considered an alternative feedstock to fossil resources for producing liquid hydrocarbons. The CO2 hydrogenation reactions were conducted over Na-FeZrOx at 330 ℃, 3.5 MPa, H2/CO2 ratio of 1:1 and 1:3, and gas hourly space velocity (GHSV) of 4000 mL g −1 h −1 . The Na-FeZrOx-9 catalyst with a Fe/Zr ratio of 9:1 exhibited extremely high C5+ liquid hydrocarbon selectivity of 79.1% (excluding CO) at a CO2 conversion of 26.3%, while the selectivity of CO (13.5%), CH4 (4.2%), and C2–C4 (14.5%) was suppressed. As the H2/CO2 ratio increased from 1:1 to 1:3, the CO2 conversion increased to 44.0% with C5+ selectivity of 58.5% with little increase in CH4 up to 14.0%. The comparison between bimetallic Na-FeZrOx-9 and other mono-metallic oxides (Fe2O3, ZrO2, and Na-Fe3O4) was also conducted. The Na-Fe3O4 catalyst showed comparatively low CO2 conversion (13.5%) and C5+ selectivity of 57.1% at a H2/CO2 ratio of 1:1. During the reaction, Fe3O4 was an active site for the reverse water gas shift reaction whereas, Fe5C2 was an active site for C–C coupling reaction. Moreover, ZrO2 acted as an electronic promoter to boost the CO2 conversion and reduced the CO selectivity. NAP-XPS analysis revealed the higher binding energy shift during the CO2 hydrogenation reaction. Furthermore, the operando DRIFTS analysis elaborated the reaction mechanism (associative mechanism) over FeZrOx-9.

Biography:

Muhammad Kashif khan has completed his PhD. degree from Sungkyunkwan University, South Korea from School of Mechanical Engineering in 2018 under the supervision of Professor Jaehoon Kim. He started his postdoctoral researcher in the same university in the field of catalytic conversion of carbon dioxide, and biomass feedstocks and unconventional crude oil upgrading. In 2020, he awarded Korea's most prestigious fellowships KRF and then NRF in 2021. Currently, he is working as a Research Professor in Sungkyunkwan University. His research work focuses on the thermo-chemical and electrocatalytic conversion of CO2 into value -added chemical by bimetallic oxides and hierarchical zeolites.

Activity of Ni/TiO_2 catalysts for electrochemical oxygen reduction reaction in alkaline media

Izabela I. Rzeznicka[1]*

Ewa Kowalska[2]
Ridwan P. Putra[1]
Hideyuki Horino[3]

[1]Shibaura Institute of Technology, Japan
[2]Institute for Catalysis, Japan
[3]Tohoku University, Japan

Abstract:

Electrochemical oxygen reduction reaction (ORR) plays a key role in a number of emerging energy conversion technologies; such as metal-air batteries and polymer membrane electrolyte fuel cells. Platinum-based catalysts have superior catalytic activity towards ORR but their high cost and deactivation over the time call for developing a stable and efficient ORR electrocatalyst based on non-precious metals. Transition metals oxides have not been considered as good electrocatalysts due to their poor electric conductivity and reactivity. In recent years however, it has been shown that a defective TiO_{2-x} exhibits high ORR activity.[1)] Here, we explored activity of Ni/TiO_2 catalysts towards ORR in alkaline solutions. The catalysts, with different nickel loadings, were prepared by photodeposition method, and commercial P25 Degussa TiO_2 was used as a support. The ORR performance was investigated by a linear sweep voltammetry (LSV) using the rotating disk electrode (RDE) method, under oxygen saturated conditions in 1 M KOH solution. The electron transfer number, obtained from the Koutecky-Levich plot, was close to 2, suggesting the $2e^-$ reduction process. The half-wave potential of the 5% Ni/TiO_2 catalyst was 0.77 V vs. RHE, which is comparable with the half-wave potential of the widely-used commercial 40% Pt/C catalyst.

Biography:

Izabela Rzeznicka studied metal-catalyzed reactions at Lodz University of Technology, Poland followed by her PhD at the Institute for Catalysis, Hokkaido University, Japan and Postdoc position in John Yates group at the University of Pittsburgh. Using sophisticated approach of the angle-resolved time-of-flight measurements of desorbing gases she identified catalytically active surface species in CO oxidation and reaction intermediates in NO reduction on Pt and Rh single metal surfaces. Her current interest is in the surface chemistry of heterogeneous processes related to renewable energy production and nanostructured systems for chemical sensing.

Oral Presentations

Highly Dispersed Metal Nanoparticle Catalysts Prepared by Atomic Layer Deposition

Xinhua Liang*

Department of Energy, Environmental & Chemical Engineering, Washington University in St. Louis, St. Louis, MO

Abstract

Normally, heterogeneous catalysts consist of small metal particles dispersed on a high surface area porous oxide support. Atomic layer deposition (ALD) is a thin film growth technique based on sequential, self-limiting surface chemical reactions, and has focused principally on the formation of thin film oxides with precise atomic layer control. Recently, ALD has been used to prepare highly active, highly dispersed metal nanoparticles. In this presentation, I will introduce ALD chemistry, metal and bimetallic nanoparticles prepared by ALD, and examples of nanostructured catalysts prepared by ALD, such as thermally stable size-selective catalysts.

Biography:

Xinhua Liang is a Professor in the Department of Energy, Environmental & Chemical Engineering at Washington University in St. Louis. He joined WashU in August 2022 from Missouri University of Science & Technology, where he was the Linda and Bipin Doshi Associate Professor of Chemical and Biochemical Engineering and had been a member of the faculty since 2012. He attended the Chemical Engineering program at Tianjin University, earning bachelor's degree in 2001 and master's degree in 2003. He received Ph.D. in Chemical Engineering from the University of Colorado Boulder in 2008 and had three years of postdoctoral training there.

Silicon Electrochemistry for Sustainable Energy Solutions

Eimutis Juzeliūnas*
Putinas Kalinauskas
Konstantinas Leinartas
Laurynas Staišiūnas
Asta Griguceviči enė

Centre for Physical Sciences and Technology, Lithuania

Abstract

Silicon is an important material for use in numerous fields, such as optoelectronics, sensors, batteries, optical fibers, photoelectrochemical water splitting, terahertz emitters, and numerous other applications. Electrochemical processes provide an opportunity to store or produce electricity with a minimum carbon footprint. Silicon electrochemistry can significantly contribute to low-carbon economy. This field offers advancement in sustainable energy solutions and environmentally friendly technologies. This presentation reports recent achievements in silicon electrochemistry, highlighting subjects of technological significance and future perspectives. The presentation features the following fields of research: (i) electrochemical silicon extraction, purification and processing in high temperature molten salts; (ii) photoelectrochemical deposition of thin silicon layers from ionic liquids; (iii) photo-catalytic effects of hydrogen generation

using silicon photo-electrodes with ultrathin oxide films (SiO_2, HfO_2, Al_2O_3); (iv) Si-oxide interfacial stability studies by the quartz crystal nanobalance – a sensitive mass detector, which provided information with nanogram resolution in situ and in real time; (v) electrochemical formation of black silicon – a nano-micro-porous material, which effectively absorbs the light in a wide range of wavelengths; (vi) outlook for the electrochemical synthesis of semiconductors, such as carbides and silicides. Advantage of electrochemical processing is discussed emphasizing environmental friendliness, technical simplicity, and cost-effectiveness.

Biography

Eimutis Juzeliūnas is a principal research associate and head of the Department of Electrochemical Materials Science at the Centre for Physical Sciences and Technology in Vilnius, Lithuania. He was a Marie Curie International Fellow of the European Commission at the University of Cambridge (UK), a Fulbright fellow at the Vanderbilt University (USA), a fellow of the American Chemical Society at the Pennsylvania State University (USA), and an Alexander von Humboldt fellow at the company DECHEMA e.V. (Germany). His recent research focuses on silicon electrochemistry for energy applications and catalysis of photo-electrochemical hydrogen generation from aqueous electrolytes.

Effect of NaOH on cellulose pyrolysis

Arjeta Kryeziu[1,2]*
Vaclav Slovak[1]

[1]Universiy of Ostrava, Department of Chemistry, Czech Republic
[2]Institut de Science des Matériaux de Mulhouse (IS2M), Université de Haute-Alsace, France

Abstract

The cellulose NaOH treatment causes a decrease in the organic and total oil yield but to the char yield increase. The NaOH treatment promote the conversion of the organic fraction into char and water. Without NaOH pre-treatment is caused elimination of levoglucosan fraction and increase of aromatic fraction.

Our aim was to explore the effect of NaOH on microcrystalline cellulose (cellulose I) and cellulosic gel materials (cellulose II) during the pyrolysis.

The carbonization process was followed by TGA under inert atmosphere at different heating rates: 2, 5, 10 and 20 $Kmin^{-1}$. Thermal degradation of samples with NaOH (CMG-NaOH and MCC-NaOH) starts earlier and are less stable than microcrystalline cellulose (MCC) and cellulosic material without NaOH (CMG). TG changes (fig. 1) are correlated with the changes in crystallinity as a function of alkalization. Where the main step of carbonization for MCC and CMG is related with one mass change, carbonization of CMG-NaOH and MCC-NaOH has complicated process of decomposition and more mass changes.

Apparent conversion degree was calculated by using Starink method.

Biography:

Arjeta Kryeziu has finished a bachelor studies for Engineering Chemistry and obtained a master degree for Analytical Chemistry and Environment. As a very motivated student, she graduated the PhD studies at University of Haute Alsace, France on the field of Materials Chemistry, and PhD at University of Ostrava, Czech Republic on the field of Analytical Chemistry. She attended several conferences such as in Brno (Czech Republic), Rome (Italy), Split (Croatia) and two other conferences on Mulhouse (France). Since PhD studies were during covid time, the attendance on the conferences was limited.

Carbon Dioxide Reduction Catalyzed by Laser-Made Nanomaterials for Sustainable Technologies

Astrid M. Müller*

University of Rochester, Rochester, NY

Abstract

Energy sustainability and green chemistry transformations require efficient and robust electrocatalytic processes to combat climate change. The accelerated discovery of new catalysts critically depends on synthetic methods that enable the preparation of tailored nanomaterials with precisely controlled properties. We show how pulsed laser in liquids synthesis can be used as a flexible synthetic strategy for efficient electrocatalysts, predicated on rational materials design. For electrolyzer devices, nanoparticulate catalysts must be immobilized on inert, high surface area carbon substrates for electrocatalysis in aqueous electrolytes. We solved this challenge by preparing structurally intact carbon fiber paper with long-lasting hydrophilicity. Our novel electrocatalysts for carbon dioxide reduction together with the newly developed ability to use them on high surface area electrode supports provide the foundation towards the realization of viable successor technologies.

Biography:

Müller is an Assistant Professor of Chemical Engineering at the University of Rochester since 2018. Prof. Müller earned a PhD in Chemistry from the Max Planck Institute of Quantum Optics, with an emphasis on ultrafast reaction dynamics. Her postdoctoral work and research as a staff scientist at Caltech centered on developing a fundamental understanding of the interactions between lasers and matter. Her independent research program is focused on the synthesis of nanomaterials using pulsed laser methods, which offer unprecedented control, uniquely positioning her to understand how composition, geometric structure, and electronic structure impact the performance of nanomaterials in electrocatalysis.

Horizontal Jet fires impinging on obstacles: simulation of flame behavior using fire dynamics simulations (FDS)

Adriana Palacios*
Pedro Castro[1]
Adriana Llante[1]

[1]Chemical, Food and Enviromental Department, Universidad de las Américas Puebla. Sta. Catarina Mártir s/n, 72810. Puebla, México.

Abstract

Jet fires are of special interest in the chemical and process industries because they can lead, essentially by domino effect, to hazardous events such as explosions, other fires or toxic gas releases. In the event of a jet fire, it is important to be able to predict its size, shape, and thermal radiation in order to foresee impingement on pipes and plates on the enclosing equipment. This paper presents a comparison of the theoretical analysis of horizontal propane jet fires (fuel mass flow rate: 0.07 kg/s) with the experimental data obtained from the simulations, using the FDS Computational Fluid Dynamics (CFD) tool software to verify the concordance of the results. The code programmed in FDS to model horizontal fire jets impinging on obstacles obtained results very similar to the experimental data. The results show behaviour, temperature profiles, and flame morphology that match and fit the experimental data. With the results of these sim-

ulations, reliable predictions can be made using the FDS software for industrial risk prevention. Despite the good results, it is important in future research to evaluate the use of other factors and models within the simulations to validate the scenarios.

Biography:

Adriana Palacios Rosas is a PhD in Chemical Process Engineering from the Polytechnic University of Catalonia. Graduated in Chemical Engineering from the Universidad de las Américas Puebla. She was part of the research staff of the Center for Technological Risk Studies of the Polytechnic University of Catalonia, carrying out the study, mathematical modeling and prediction of effects and consequences of serious fuel accidents and explosions. In charge of the project Experimental studies and mathematical and computational modeling of dart fires, as a staff researcher at the School of Mechanical Engineering, University of Leeds, United Kingdom.

Understanding the Dynamic Evolution of Dispersed Transition Metal Catalysts During Electrocatalytic CO_2 Reduction: A Combined Computational XANES and Mechanistic Study

Cong Liu*
Jiayi (Jason) Xu

Argonne National Laboratory, USA

Abstract

Direct Electrochemical conversion of CO_2 to ethanol (CH_3CH_2OH) offers a promising strategy to lower CO_2 emission while storing energy from renewable electricity. However, the high selectivity for producing CH_3CH_2OH using current electrocatalyst is rather difficult. Our recent study reported that a synthesized atomically dispersed Cu catalyst achieves high selectivity of CH_3CH_2OH of 91% with low onset potential at -0.4 V, however, the active site structure that is responsible for such high activity and the reaction mechanism have never been well understood. In this paper, we carried out computational modeling combining X-ray absorption near edge structure (XANES) simulation and first-principal density function theory (DFT) mechanistic study to investigate the catalyst structures and reaction pathways during electrocatalysis. In combination with previous experimental data, our results showed that the as-prepared Cu catalyst undergoes a structural evolution under electrochemical condition, forming Cu clusters and nanoparticles with a distribution of size. Reaction mechanism studies show that the Cu particle size effect on catalytic activity and product selectivity is remarkable and follows a trend as the size increases; smaller Cu clusters show higher activity and selectivity for CH_3CH_2OH, while intermediate particles favors CO formation, and large particles have higher selectivity for HCOOH and CH_4 formation. The theoretical findings are consistent with experimental results and further revealed catalysts structures during dynamic evolutions and reaction mechanism. The conclusions from this report can be further used as design principle to discover novel catalyst materials for CO_2 electrochemical reduction.

Biography:

Cong Liu is a Chemist in Chemical Sciences and Engineering Division at Argonne National Laboratory. She received her Ph.D. degree in Physical Chemistry at University of North Texas in 2013. She was then awarded the Argonne Director's Fellowship at Argonne. Her research has been focused on computational materials and catalyst design and computational spectroscopy. She is interested in catalytic C-H activation, C-C activation/formation, and CO_2 reduction, as well as development of battery materials. Her work has been published on Science, Nature, Nature Energy and JACS, etc.

Catalytic Biomaterials for Atrazine Degradation

Karla Diviesti[1]
Richard C. Holz[1]*

Contribution from the [1]Department of Chemistry, Colorado School of Mines, Golden, CO

Abstract

Atrazine (2-chloro-4-ethylamino-6-isopropylamino-s-triazine) is a water-soluble herbicide used extensively across the United States. Its toxicity and persistent mobility directly affects the health of aquatic communities and poses serious downstream concerns for human health. Triazine hydrolase (TrzN) from Arthrobacter aurescens TC1, is an enzyme that catalytically degrades atrazine. We recognize TrzN's potential as a biocatalyst and to date, we have successfully immobilized TrzN in alginate beads (TrzN:alginate), chitosan coated alginate beads (TrzN:chitosan), and tetramethylorthosilicate (TMOS) gels using the sol–gel method (TrzN:sol–gel). TrzN:alginate and TrzN:chitosan hydrolyzed 50 μM of atrazine in 6 h with negligible protein loss with an ~80% conversion rate. The TrzN:sol–gel biomaterial converted >95% of a 50 μM atrazine solution in an hour with negligible protein loss. The treatment of each of these biomaterials with trypsin confirmed that the catalytic activity was due to the encapsulated enzyme and not surface-bound TrzN. All three of the biomaterials showed potential for long-term storage and reuse, with the only limitation arising from the loss of protein in the storage buffer from TrzN:alginate and TrzN:chitosan. Additionally, the materials stayed active in methanol concentrations <10%, suggesting the ability to increase the solubility of atrazine with organic solvents. The structural integrity of the TrzN:alginate and TrzN:chitosan materials became limiting in extreme pH conditions, while TrzN:sol–gel outperformed WT TrzN. Overall, the TrzN:sol–gel biomaterial proved to be the best biocatalyst and insights into immobilizing TrzN and our pursuit of utilizing TrzN as a biocatalyst for atrazine bioremediation will be discussed.

Biography:

Karla Diviesti is currently a 4th year PhD candidate in the Quantitative Biosciences and Engineering interdisciplinary program at the Colorado School of Mines. Her research focuses on uncovering the catalytic mechanisms of hydrolytic dehalogenases and utilizing those enzymes in a variety of biomaterials. In 2022 Karla was inducted into the scientific research honor society Sigma XI. Prior to attending Mines, Karla attended Clemson University and studied biosystems engineering with an emphasis in bioprocess engineering.

Interplay Between Local Structure and Nuclear Dynamics in Tungstic Acid: a Neutron Scattering Study

Matthew Krzystyniak[1]*
Kacper Druzbicki[2]
Erwin Lalik[3]
Gavin Irvine[4]
Matthias Gutmann[1]
Svemir Rudic[1]
Pascal Manuel[1]
Vaclav Petricek[5]

[1] ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, OX11 0QX, United Kingdom
[2] Polish Academy of Sciences, Lodz, Poland
[3] Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences; Poland

[4] School of Chemistry, University of St Andrews, St Andrews, Fife KY16 9ST, United Kingdom
[5] Institute of Physics, Czech Academy of Sciences, Na Slovance 1999/2, Praha 8, 182 21, Czech Republic

Abstract

We provide an exhaustive characterization of structural properties and nuclear dynamics in tungstic acid (WO3·H2O). To this end, we employ Neutron and X-ray Diffraction (ND and XRD) combined with Inelastic Neutron Scattering (INS) and Neutron Compton Scattering (NCS) and corroborate the analysis with extensive ab initio modelling. The ND and XRD results are confronted with low-temperature INS experiments and zero-temperature phonon calculations. The analysis reveals an inconsistency in the definition of the structure of confined water with respect to crystallographic data, also showing a concomitant fail of the phonon calculations due to a strongly anharmonic confining potential. Extending the computational route toward ab initio MD (AIMD) simulations allows us to probe different structural configurations and provides an improved description of the vibrational dynamics as compared to highresolution INS experiments, nevertheless, requiring the use of effective classical temperatures. The analysis of both INS and the NCS data reveals a remarkable similarity to the nuclear dynamics earlier reported for water confined in Single-Wall Carbon Nanotubes (SWNT), which has been qualitatively described as a new phase of ice. Our analysis reveals a strong two-dimensional hydrogen-bonding network, similar to the shell model for water in SWNT. The reported NCS data show narrowing of the hydrogen momentum distribution with respect to the reference ab initio calculations, indicating a great deal of conformational freedom due to spatial delocalization of protons in the ground state of the system, a clear signature of the quantum character of the nuclei.

Biography:

I received a Master of Physics and PhD in biological nuclear magnetic resonance (NMR) at the Jagellonian University in Cracow, Poland. I continued my research career in biological NMR and electron paramagnetic resonance (EPR) as a postdoctoral research associate at the Free University of Berlin, University of Durham and Oxford. In 2003, I started working on the applications of neutron Compton scattering (NCS) in nuclear chemical dynamics of condensed matter systems and molecules. In 2015, I obtained a position as an instrument scientist in electron volt neutron spectroscopy at the ISIS Neutron and Muon Source, UK.

X-ray spectroscopy for advanced investigation of energy materials

Chung-Li Dong[1]*

[1]Department of Physics, Tamkang University, Taiwan

Abstract

In response to the worldwide surge in energy demand, the materials scientists devote themselves to the search for clean and sustainable energy. Without the development of cutting-edge renewable energy materials, going green has never been simple. The zero-emission future requires a multifaceted approach. Advanced functional materials for more effective energy conversion, storage, and conservation are the universal focus of energy research. Although the ideas for increasing the efficiency of current energy materials in terms of energy conversion, storage, or conservation are clear and straightforward, they are technically challenging. It is difficult to better engineer materials in an efficient manner for a practical use without knowing the fundamental atomic and electronic structures, particularly how they respond under operating conditions. Synchrotron x-beam spectroscopies, including x-ray absorption and emission spectroscopies are powerful tools to study the local unoccupied and occupied electronic states.

In addition, employing the in situ technique permits us to monitor the atomic and electronic structure modulations of the energy material at work. An emerging x-ray spectro-microscopic technique, scanning transmission x-ray microscopy, which provides spatially resolved x-ray spectroscopy. The significance of utilizing x-ray spectroscopy for the atomic and electronic structure characterization of several significant energy material systems, such as advanced nanocatalysts, artificial photosynthesis materials, and smart materials, will be discussed in this presentation. Recent developments of in situ technique, a number of recent studies, and energy science-related Tamkang University (TKU) end-stations at the BL45A and BL27A of the Taiwan Photon Source (TPS) will also be presented.

Biography:

Chung-Li Dong holds a PhD in physics from Tamkang University in 2004. Between 2005 and 2009, he worked as a postdoctoral researcher at Institute of Physics at Academia Sinica in Taiwan, and Advanced Light Source at Lawrence Berkeley National Laboratory in the United States. He worked as a scientist at National Synchrotron Radiation Research Center (NSRRC) in Taiwan from 2009 to 2015. Currently, he is a professor at Research Center for X-ray Science and Department of Physics, Tamkang University. His research work now focuses on the synchrotron-based and in situ/operando spectroscopic studies of advanced and energy materials.

Multifunctional Carbon-based Metal-free Catalysts for Energy/Environmental Applications

Hyoung-il Kim*
Haein Cho
Do-Yeon Lee
Zeeshan Haider

Department of Civil and Environmental Engineering, Yonsei University, Korea

Abstract

Multifunctional carbon-based metal-free catalysts have been in the frontier of chemical engineering and material science involving graphene, carbon nanotubes, buckyballs, carbon quantum dots, and carbon nitrides, as they involve appealing characteristics such as chemical stability, high-degree of surface functionality with catalytic and photo-responsible reactivities. Herein, we introduce various strategies for designing multifunctional carbon-based metal-free catalysts for specific energy/environmental catalytic reactions. With various applications, (photo or electro)catalytic production of hydrogen peroxide (H_2O_2) with multifunctional carbon-based metal-free catalysts has been considered as one of the most promising catalytic systems because its production requires only sunlight, water, and air. Thus, a couple of examples for the purpose-designed carbon-based catalysts for (photo or electro)catalytic production of H_2O_2 will be introduced. We will also provide studies with the purpose-designed carbon-based catalysts for other applications including solar hydrogen production and reactive oxygen species generation for water purification.

Biography:

Hyoung-il Kim is the Hwalchun Endowed Professor in Department of Civil and Environmental Engineering at Yonsei University. He received his Ph.D and M.S. in School of Environmental Science and Engineering at Pohang University of Science and Technology. He then moved to Yale University for two and a half years as a postdoctoral research fellow. His research expertise resides in solar-driven catalysis for water-energy nexus, combined with advanced oxidation processes (AOP), solar fuel production, and (photo)electrochemical wastewater treatment.

Precious Metal Catalysts for the Conversion of Sustainable Feedstocks

Chiranjit Sapre

Heraeus Precious Metals

Abstract

Although fossil feedstock was and is the predominant feedstock for the chemical industry, renewable feedstocks are alternatives to fossil resources. The aim is to reduce the carbon footprint and open up new routes to platform chemicals.

Forestry residues, such as lignin or 5-hydroxymethylfurfural (HMF) from cellulose, can serve as a renewable source of value-added chemicals. To date, lignin has been used primarily in paper manufacturing as an energy source, although it can also be used as a valuable feedstock for the chemical industry. Lignin is one of the most abundant polymers in nature and contains a variety of aromatic components.

In this presentation, we highlight strategies for obtaining organic building blocks and platform chemicals from renewable feedstocks by the effective deployment of precious metal-based catalysts. We describe in an use case, the development of a platinum-based catalyst for the efficient formation of phenolics from lignin for the use in phenolic resins. Both platinum loading and the selected support material influence the catalyst performance. The use of the optimized platinum-based catalyst ensures access to the organic building blocks while completely avoiding any coke formation.

Furthermore we will also discuss the cost attractiveness of precious metal-based catalysts, when applying recycling loop strategies, which allow an efficient use of the scarce precious metals.

Biography:

Chiranjit Sapre currently supports Heraeus Precious Metals commercial function for Chemical Products, Chemical Catalysts and Recycling in North America.

He has spent past 14 years in various segments of precious metals industry. He joined Heraeus in Oct of 2017 and since then has engaged with clients from a small and medium enterprises to fortune 500 companies.

Tuning electrochemical reaction kinetics through interfacial hydrogen bonding

Yirui Zhang*
Yang Shao-Horn

Massachusetts Institute of Technology, USA

Abstract

Electrocatalysis plays a key role in fuel cells and decarbonation. Conventional design has focused on tuning the surface electronic structures of catalysts and binding strength of intermediates, while recent studies show that changing electrolyte compositions, such as spectator cations and pH, can also significantly alter catalytic kinetics by orders of magnitude, highlighting new opportunities in electrolyte engineering to control catalytic activities. We have recently demonstrated tuning the oxygen-reduction reaction (ORR) kinetics through an interfacial layer of protic ionic liquids, where altering the pK_a of organic ionic liquids increases the intrinsic activity by up to five times. The enhancement is attributed to the strengthened hydrogen bonding

between the ionic liquid and reaction products, supported by density functional theory (DFT) calculations and surface-enhanced infrared absorption spectroscopy (SEIRAS). We further investigate hydrogen evolution and oxidation reactions (HER/HOR) and systematically confine water in organic matrixes. We can tune the hydrogen-bonding networks by changing the water concentration and altering the donor number of organic solvents. The shifts in onset potentials are solvent-dependent, where high donor number solvents suppress HER more significantly due to its stabilization effect of isolated water, while the enhancement effect of HER with low donor number solvents is due to the promotion of interfacial hydrogen-bonded water. These findings open up immense opportunities for using non-covalent hydrogen bonding interactions at the electrified interface to control the kinetics. The understanding would also be impactful across other reactions involving proton transfer that are crucial for energy storage, such as CO_2 reduction and aqueous batteries.

Biography:

Yirui Zhang received her Bachelor's degree from Tsinghua University. She later joined Massachusetts Institute of Technology (MIT) to obtain her Ph.D. working with Professor Yang Shao-Horn, where she focused on in situ characterization and physical chemistry of interfaces for electrochemical energy storage and conversion. She will join Stanford University as a postdoctoral researcher starting Fall 2022. She has co-authored 26 peer-reviewed articles in journals including Nature Catalysis and Energy & Environmental Science.

The Effect of Titania Covering: Retarding the RWGS Reaction in Selective CO Methanation

David Kumi[a]
Neil Coville[b]

[a]Department of Physics and Engineering Science, Coastal Carolina University South Carolina.
[b]Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, RSA

The possible commercialization of proton exchange membrane fuel cells (PEMFCs) depends on reducing the concentration of CO in the reformate gas through viable methods, such as selective CO methanation [1]. We report on hindering the undesired reverse water gas shift (RWGS) reaction that occurs during selective CO methanation, by using a nano-Ru catalyst supported on TiO2 coated CNTs (Ru/CNT-TiO2). The Ru catalyst (5%wt) was loaded onto CNT-TiO2 and other carbon supports

(CNT and N-CNTs via wet incipient impregnation and microwave polyol methods.

Coating carbon with TiO2 significantly improved the surface area and enhanced the thermal stability of the coated catalyst. In addition, the coated support severely retarded the progress of the undesired reverse water gas shift reactions (RWGS) that was pronounced in the carbon supports. The carbon supported catalysts without TiO2 showed lower catalytic activity in terms of CO

methanation compared to its TiO2-coated analogue (5%Ru/CNT-TiO2). This was attributed to the synergy between the carbon and titania in the composite, which resulted in an improved dispersion of active sites leading to higher activity [2].

Recovery of hydrocarbons from organic wastewaters by catalytic hydro-de-hetero-atoms under hydrothermal conditions

Shetian Liu*
Dandan Mu
Dongwei Li
Zhuwan Li
Yong Liu
Siyu Yu

School of Chemistry and Chemical Engineering, Southwest University, China

Abstract

The removal of harmful heteroatoms from organic wastewaters or waste liquids often requires stringent reaction conditions, such as high temperature incineration, supercritical water treatment, thermal plasma gasification and so on. It is of great economic value to recover hydrocarbons from toxic and harmful organic pollutants by catalytic hydro-de-heteroatom (HDH) reactions under mild hydrothermal conditions. Some typical reactions have been studied recently in our laboratory focusing on the development of efficient and hydrothermally stable catalysts for commercially feasible HDH processes. These studies include but not limited to the deoxygenation of Fischer-Tropsch (FT) synthesized water, hydrodechlorination of chlorobenzenes, and hydrodenitrogenation of nitrobenzene, in combination with the aqueous phase reforming (APR) of methanol to supply hydrogen. The progress of our research work includes: 1) near-complete removal of oxygenates from the FT water with supported ruthenium catalysts for fuel gas recovery; 2) greatly improved stability of a nickel-based catalyst for APR of methanol; 3) selective hydro-denitrification of nitrobenzene to cyclohexanone. A common obstacle encountered is the catalyst deactivation under the hydrothermal reaction conditions. Growth of metal particles, surface reconstruction, and/or phase transformation of key components of the catalysts by the hydration/hydrolysis action in aqueous phase are the challenges faced academically and technically in the industrial catalyst development. This presentation is to share with colleagues our latest research results and discuss the problems and countermeasures in the development of HDH technologies.

Biography:

Shetian Liu is a Distinguished Professor in the School of Chemistry & Chemical Engineering, Southwest University, China. He received his PhD in 1993 from Changchun Institute of Applied Chemistry, Chinese Academy of Sciences (CAS). He worked as scientist and research engineer in internationally renowned energy and manufacture companies and institutions, including ConocoPhillips Company, IHI Corporation, and Dalian Institute of Chemical Physics, CAS. He has more than 100 peer-reviewed journal papers, patents, and internal technical reports. His research covers catalysis for natural gas conversion, hydrogen production, automotive emission control, wastewater treatment, and catalysis for petroleum refining and coal chemical industries.

Engineering RNA as anion polymers for programmable self-assembly of nanostructures for applicators in the fields of medicine and materials

Kai Jin*
Daniel Binzel
Dan Shu
Peixuan Guo

Center for RNA Nanobiotechnology and Nanomedicine, Division of Pharmaceutics and Pharmacology, College of Pharmacy; Comprehensive Cancer Center, College of Medicine.
The Ohio State University, US.

Abstract

The importance of polymers for application in the fields of medicine and materials has received considerable attention due to their broad applications. RNA, although it was previously thought to be unstable, has been found to possess unique properties that make it a suitable material for the importance of polymers for applicators in the fields of medicine and materials has received considerable attention in recent years due to their potential applications. RNA, although it was previously thought to be unstable, has been found to possess unique properties that make it a suitable material for building nanostructures, including, triangles, cubes, prisms, pyramids, hexagons, arrays, bundles, membranes, and microsponges. This was made possible by modifications to render RNAs resistant to degradation while retaining their programable folding and self-assembly properties with unique biological functions. The discovery of ultra-thermostable RNA 3WJ motifs facilitates the application of RNA. Interest in the emerging field of RNA nanotechnology has increased significantly in recent years, as evidenced by more than a thousand publications in different fields. The popularity of RNA nanoparticles can be attributed to several factors, including but not limited to their high thermodynamic stability, ability to control shape, size, and stoichiometry, and there, and as a safe and disease-specific treatment modality. Besides the application in the delivery of therapeutics for cancer intervention, which is my focus of the presentation, the application of RNA as nanomaterials for logic gates, resistive memory, and biomedical sensing will also be discussed.

Biography:

Kai Jin graduated from Fudan University with a bachelor's degree in Biotechnology in 2018. After that, he received his master's degrees from the University of Pennsylvania in Bioengineering and Computer and Information Technology in 2021. Before joining Dr. Peixuan Guo's lab, he worked with Dr. Zhiqing Pang at the School of Pharmacy, Fudan University on brain-targeting drug delivery platforms. Currently, he is a second-year Ph.D. student in the School of Pharmacy, the Ohio State University working on RNA Nanotechnology.

Advancing asymmetric light-mediated Ni catalysis using data science and physical organic techniques

Ana Bahamonde*
Robert Bradley
Brennan McManus
Olivia Taylor
Hung Lang Cheng

University of California Riverside, USA

Abstract

The Bahamonde group harnesses the distinct one-electron chemistry and photochemical reactivity of Ni complexes to generate and trap C-centered radicals enantioselectively and promote C–N reductive eliminations at room temperature. Our excitement for studying these systems stems from the fact that these two apparently unrelated processes are facilitated under almost

identical conditions, but to date the ligand features, photocatalyst properties, and subtle reaction condition variations that favor one pathway over the other are not yet understood. Additionally, to expedite reaction optimization, the group develops multivariate linear regression models correlating observed enantioselectivity to computed molecular descriptors.

Biography:

Ana did her PhD in the Melchiorre lab (ICIQ), where she studied photoredox reactions promoted by organocatalysts. Then she joined in the Sigman group as a postdoc where she worked on Pd-catalyzedaza-Wacker reactions and the development of multivariate linear regression models to explain of amide coupling rates. Since 2020, Ana is an Assistant Professor at the University of California Riverside where her group uses a mechanistically guided approach to reaction development utilizing first row transition metals.

Turning glycerol to value-added chemicals in the absence of external hydrogen over copper catalysts supported on SBA-15-type materials containing zirconium

Julio Colmenares-Zerpa[1,2]
Jorge Gajardo[1]
A.F. Peixoto[3]
F. Gispert-Guirado[4]
J. Llorca[5]
R.J. Chimentão[1*]

[1]Universidad de Concepción, Chile
[2]Universidad de Los Andes, Venezuela
[3]Universidade do Porto, Portugal
[4]Universitat Rovira i Virgili, Spain
[5]Universitat Politècnica de Catalunya, Spain

Abstract

Several routes have been explored for the glycerol valorization to high value-added chemicals. Herein, the glycerol conversion over copper catalysts supported on SBA-15-type mesoporous materials was evaluated in a batch reactor at 220 °C under N_2 atmosphere. Zr-SBA-15 (Si/Zr=∞, 10, 5, and 2) supports were prepared by the pH adjustment method. Copper catalysts were prepared by the incipient impregnation method. N_2-physisorption and X-ray diffraction (XRD) indicated that the catalysts come up with mesoporosity. High-resolution transmission electron microscopy (HRTEM) revealed that the Zr introduction in the supports generated a gradual loss of long structural ordering. In addition, larger copper particle sizes were obtained over the catalysts containing a higher Zr load. X-ray photoelectron spectroscopy (XPS) of the as-prepared catalysts indicated a higher atomic surface Cu/Si ratio as the Zr load increased. The absence of external and internal diffusional limitations was verified by applying the Mears and Weisz-Prater criteria. The highest values of specific initial rate and rate constant were obtained in catalysts with zero or low Zr loading. Hydroxyacetone (HA) and 1,2-propanediol (1,2-PDO) were the main formed products. Hydroxyacetone formation reached a maximum of 90% selectivity along the reaction meanwhile, 1,2-PDO achieved a progressive evolution with time until 10% selectivity. Initial formation rates of HA and 1,2-PDO were optimized in the copper catalyst containing the lowest Zr load. The formation of 1,2-PDO in the absence of external hydrogen is highlighted. In conclusion, the Zr load in the copper catalysts is a regulating parameter of textural, structural, acidic, surface, and catalytic properties.

Biography:

R.J. Chimentão graduated in Chemical Engineering at the State University of Campinas (Unicamp, Brazil) in 1999. At Unicamp, He received his Master´s degree in 2002. In 2007, He received his Ph.D. degree from the Universitat Rovira i Virgili (Spain). Between 2007 to 2016 He was a postdoctoral fellow in different research centers: CNRS (France), Purdue University (USA), LNLS (Brazil), and the Laboratory for Chemical Technology at the Ghent University (Belgium). He was Assistant Professor at the Faculty of Chemical Sciences of Universidad de Concepcion (Chile) from 2016 to 2022 and at present, he became an Associate professor.

Renewable Sources for the Production of Sustainable Clean Fuels: Need of Catalysts, or Not?

Youssef Berro

PROMES-CNRS, France

Abstract Not Available!!!

What are the Oxidizing Intermediates in the Fenton and Fenton-Like Reactions? A Short Review

Dan Meyerstein

Ariel University, Israel

Abstract Not Available!!!

Advanced Catalysts to Decarbonize Our Future?

Mohammad Asadi

Illinois Tech, Chicago, IL

Abstract Not Available!!!

Reductive amination of carbonyl compounds from Biomass feedstocks. A catalytic green route for synthesis of primary amines and Amino Acids

Doris Ruiz*
Karen Morales2
Mario Sáez3
Jordan Carrasco4
Universidad de Concepción, Chile

Abstract

Amino acids (AA) are the basic building blocks of protein synthesis and for this reason are widely used in the field of biological, pharmaceutical, food and industrial medical intermediates. Currently the production of AA is mainly obtained via biocultivation process and by the way of chemical methods. In both cases, the severe operation conditions and complicated separation procedures show some restrictions on industrial application. Therefore, developing new process for efficient amino acid production via a green and clean way is of significance but still an open challenge.

This study describes the synthesis of amino-compounds from Biomass-derived chemicals, specifically compounds containing oxygen groups which can be used as a renewable feedstock. The reductive

amination of compounds from biomass-derivative substrates with NH3 is a process that meets with the demand of economical and greener processes in AA production through reductive amination.

All reactions were carried out using Rh based catalysts. Rh materials were synthesized by wet impregnation and characterized by N2 sorption, Chemisorption, XPS, XRD, SEM, TEM, NH3-TPD and TPRH2. The reaction conditions also affect the process and therefore the reaction temperature, the substrate/metal molar ratio and the gas pressure in the feed were studied. The best reactions conditions parameters were 373 K, 4 bar of NH3, 2 bar of H2, using a substrate/Rh mol ratio=100 and other reactions conditions were at 800 rpm in 50 mL of cyclohexane. Products of reaction were analyzed by GC-MS. The catalysts were active and selective in hydrogenation and amination reactions of acetophenone, lactic acid and cyclohexanone. The conversion to amines can be affected by metallic diameter, metal dispersion and metal reduction ratio, among others. Conversion of ketones involves amination and hydrogenation steps to produce high conversion and maximum selectivity (100%) to primary amines. Lactic acid showed conversion to alanine by successive dehydrogenation-amination-hydrogenation pathways of reaction.

Biography:

Doris Ruiz is currently Associate Professor in Physical Chemistry at the University of Concepcion, in Concepción, Chile. She has her expertise in Heterogeneous Catalysis, specifically focused on:

Enantioselective Catalysis, Hydrogenation and Amination reactions, valorization of compounds from Biomass feedstocks, Green Chemistry, Fine Chemistry and Nanomaterials. She leads the “Laboratory of Heterogeneous Catalysis for Valorization and Selective Chemical Processes”. She currently focuses her research on the catalytic synthesis of amino acids from α-hydroxy acids obtained from biomass feedstocks over supported bimetallic catalysts.

Direct Conversion of Methane to Value-Added Hydrocarbons using Hybrid Catalysts of Ni/Al2O3 and K-Co/Al2O3

Anusorn Seubsai

Kasetsart University, Thailand

Abstract Not Available!!!

Coupling of Alternating Current to Transition-Metal Catalysis

Sergey N. Semenov*
Evgeniy O. Bortnikov

Weizmann Institute of Science, Israel

Abstract

Catalysis is the key element for a sustainable chemical industry. Transition-metal catalysis is among the most developed forms of catalysis. Nevertheless, classical transition-metal catalysis has some fundamental limitations: (i) as for any catalysis, only thermodynamically favorable reactions can be enabled; (ii) some steps (e.g., oxidative addition to Cu(I)) are too slow for effective catalysis. Both problems could be overcome by coupling transition metal catalysis to an external source of energy. Examples of coupling transition-metal catalysis to light and direct current (DC) electrolysis are common in the literature. In this work, we demonstrate a new approach to catalysis based on the coupling of alternating current (AC) to transition-metal catalysis. AC-assisted Ni-catalyzed amination, esterification, and etherification of aromatic bromides showed higher yields and selectivity compared to observed in the control experiments with direct current (DC). The use of AC allows oxidation and reduction to occur on the same electrode and provides three important advantages: (i) it obviates the need to transfer reactive intermediates between electrodes, which prevents the intermediates' dilution, allows working with short-living intermediates, and opens up opportunities to scale-up synthesis using porous electrodes without mixing; (ii) the use of the frequency and the waveform of AC as easily tunable experimental parameters; (iii) the possibility to achieve potentials beyond the solvent electrochemical window if the electron transfer rate to/from the solvent is much slower than the electron transfer to/from the catalytic metal. The AC assistance should be well-suited for catalytic cycles involving reductive elimination or oxidative addition as a limiting step.

Biography:

Sergey Semenov earned a master's degree in chemistry with honors from Moscow State University, Russia in 2006. He earned a PhD in chemistry with honors from the University of Zurich, Switzerland in 2011. He started postdoctoral work in the group of Prof. Wilhelm Huck at the Radboud University of Nijmegen, The Netherlands in autumn of 2010, and became a Marie-Curie fellow in 2012. From 2014 to 2017, he was a postdoctoral scholar in the group of Prof. George Whitesides at Harvard University. In 2018, he became a principal investigator at the Weizmann Institute of Science, Israel.

Synthesis of Cu Nanosheets on Macroporous Ni-GO Skeleton in Application of Wire-Like Supercapacitors with High Energy Density

Ruitao Zhou

Hong Kong Polytechnic University, Hong Kong

Abstract Not Available!!!

Stability and ion pairing of alkalides in organic solutions

René Riedel[1]*
Andrew G. Seel[2]
Daniel Malko[3]
Daniel P. Miller[4]
Brendan T. Sperling[4]
Heungjae Choi[5]
Thomas F. Headen[2]
Eva Zurek[6]
Adrian Porch[5]
Anthony Kucernak[3]
Nicholas C. Pyper[7]
Peter P. Edwards[8]
Anthony G. M. Barrett[3]

[1] University of California, Riverside, USA
[2] ISIS Neutron and Muon Source, U.K.
[3] Imperial College London, U.K.
[4] Hofstra University, USA
[5] Cardiff University, U.K.
[6] State University of New York at Buffalo, USA
[7] University of Cambridge, U.K.
[8] University of Oxford, U.K.

Abstract

Alkali metal solutions comprising alkali metal anions, the 'alkalides', and complexed alkali cations side by side provide a large untapped potential with respect to future applications. This is due to their unique properties such as a strongly reducing nature and a high polarizability. The use of organic complexing agents such as crown ethers and cryptands allows for the stabilization of high concentrations of charge carriers in a weakly polar medium. Nevertheless, the currently available knowledge about those solutions is very limited and their characterization is mostly centered around alkali metal NMR techniques. A significant upfield shift and exceptionally narrow width of the alkalide NMR signal were ascribed to the high shielding and symmetry of an effectively unperturbed 'gas-like' anion in solution with little to no interaction with its local environment.

Our investigations extend this traditional picture of the alkalide in solution and unveil the underlying effect of Coulomb interactions on the properties of alkalides in low-polarity solvents by a comprehensive combination of spectroscopic methods. Concentration dependent measurement of both conductivity and permittivity of alkalide solutions revealed that ion pairing is a key factor in determining their kinetic properties and stability. Furthermore, the effect of dissolved metal on the mesoscopic structure of solutions of macrocyclic complexants is probed by small angle neutron scattering. Ultimately, we present a rationale for the rather obscure and unexpected temperature- and concentration-dependence of alkali metal dissolution in organic media and provide a multi-facetted understanding of the remarkable preparatory and spectroscopic characteristics of alkalide solutions.

Biography:

René Riedel grew up in Bavaria, Germany, and obtained his M.Sc. in Chemistry from FriedrichAlexander-University Erlangen-Nuremberg. In the course of his PhD project under the supervision of Professor Anthony G M Barrett at Imperial College London, he established several research collaborations focusing his interest on alkali metal solutions and their synthetic applications. Since he joined Professor Richard R Schrock's group at UC Riverside he studies the formation of alkylidene complexes from olefins under the influence of visible light.

Template-assisted synthesis of single-atom catalysts supported on highly crystalline vanadium pentoxide for stable oxygen evolution.

Ki Ro Yoon*

Advanced Textile R&D Department, Korea Institute of Industrial Technology, South Korea

Abstract

The concept of single-atom catalysts (SACs) as heterogeneous electrocatalysts has received growing attention due to their high catalytic activity, maximized atomic utilization, and cost efficiency. However, the use of SACs in practical applications has still encountered challenges with regard to the corrosive environment of carbonaceous support materials, resulting in underwhelming durability of catalysts.

We present an unprecedented synthetic approach to prepare highly crystalline Co-doped vanadium pentoxide for stable oxygen evolution reaction. The large exposure of Co atomic sites in highly ordered layered oxide successfully enables effective binding with reaction intermediates, resulting in operational activity and exceptional durability. This work will open up a larger opportunity for the organic-template-assisted synthesis of novel SACs and suggests that the combination of high-crystalline oxide supports could be a crucial approach to enhancing both activity and stability.

Biography:

Ki Ro Yoon started as a senior researcher of Advanced Textile R&D Department at KITECH in December 2018. He was appointed adjunct professor of HYU-KITECH joint department in Hanyang University since November 2021. He received his Ph.D. in department of Materials Science and Engineering from KAIST in February 2018, and served as a postdoctoral fellow at the KIST until November 2018. His current research is focused on the development of nanomaterials and membranes for electrochemical energy and environmental applications.

Exploiting Subnanometer Cluster Size, Atomic Composition and Support Effect in Selective Dehydrogenation and Hydrogenation Reactions

Stefan Vajda

J. Heyrovský Institute of Physical Chemistry, Czech Republic

Abstract Not Available!!!

IL Properties of Yttrium-Doped Barium Titanate for High Performance Multilayer Ceramic Capacitors

Mohammed Tihtih

Institute of Ceramic and Polymer Engineering, Hungary

Abstract Not Available!!!

Keynote Presentation

Potential Hybrid Catalysts for CO2 Reactions

Martin Schmal

Federal University of Rio de Janeiro, Brazil

Abstract Not Available!!!

Oral Presentations

Nanoscaled Silicon Carbide on Silicon: A New Bandgap Material for Micro- and Optoelectronics and its Unique Properties

Sergey Kukushkin

Institute of Problems of Mechanical Engineering, Russia

Abstract Not Available!!!

Metal- and acid-free activation of carbonyl moiety – Esterification of Aryl/Alkyl acids catalyzed by N-halamines

Bojan Božić[1]*
Klara Čebular[2]
Jelena Lađarevi[3]
Miloš Petković[4]
Dušan Mijin[3]
Stojan Stavber[2]

[1] University of Belgrade, Institute of Physiology and Biochemistry "Ivan Djaja", Faculty of Biology, Serbia.
[2] Jožef Stefan Institute, Department of Physical and Organic Chemistry, Slovenia.
[3] University of Belgrade, Faculty of Technology and Metallurgy, Serbia.
[4] University of Belgrade, Faculty of Pharmacy, Serbia

Abstract

In recent decades, environmental awareness is growing, along with the demand for eco-friendlier technologies, which consequently act as a main driving force for exploration and development of greener methodologies. N-halamines are well-known as convenient, easily manipulable and low-priced halogenation reagents in organic synthesis. In the past decade, these compounds have been placed in a completely new context –as acid- and metal-free catalysts. The activation of carbonyl moiety and its susceptibility toward the nucleophilic attack affords the construction of various organic compounds, representing one of the most rudimentary approaches to organic synthesis which is crucial for a plethora of industrial-scale condensation reactions, such as esterification. The existence of oxygen lone pairs puts the carbonyl moiety into the context of a Lewis base, prone to activation in the presence of a Lewis acid, which has already been extensively studied. Halogen bonds – noncovalent interactions – provided by

halogen atoms in haloorganic compounds can be assumed responsible for the catalytic activity of different N-halamines under diverse reaction conditions (conventional heating or microwave irradiation). Thereby, exploring N-halamines from this novel perspective holds promise for substantial advances in organic synthesis. Within this, an optimal reaction method (where the carbonyl moiety activation represents an essential step) should meet the following criteria: 1) an easily-manipulable, low-cost, non-metal, water- and air-tolerant catalyst, 2) mild and/or solvent-free reaction conditions, 3) no need for simultaneous water removal, and, 4) stoichiometric amounts of activators or large excesses of reagents.

Biography:

Bojan Božić – Senior Research Associate with research experience in the field of Organic Chemistry and Bioinformatics. BB holds a PhD degree in Chemical Engineering and two postdocs. BB was a member of evaluation board for 4 doctoral theses, and more than 20 master and specialization theses. BB has participated in 7 national/international projects, and one COST action. Over the career, BB scientific output comprises 55 papers published in SCI-journals, cited more than 550 times (h-index–15, i-index–27, source: Google Academic). BB was awarded from the "Start Up for Science" program, supported by Phillip Morris for his original research concepts.

Catalytic Conversion of CO_2 over CeO_2 based Catalysts

Parisa Ebrahimi
Anand Kumar*
Majeda Khraisheh

Department of Chemical Engineering, Qatar University, Qatar

Abstract

Herein, a report the synthesis and catalytic performance of Cu, Ni supported catalyst on CeO_2 for CO_2 catalytic conversion to carbon monoxide and methane. The catalysts were synthesized using combustion synthesis technique to obtain high dispersion of metals, which were loaded to 1wt% value. The catalysts support, CeO_2, were also synthesized together with the metal using the same technique. In addition, commercial CeO_2 support was also used for comparison purpose, along with the combustion synthesized CeO_2 support. In a typical synthesis process, the precursors nickel-nitrate, coper-nitrate and cerium nitrate are dissolved in water and combusted in presence of a fuel glycine/urea and the resulted powders are collected and used as supported catalyst. The catalysts are then calcined at various temperatures, 400 °C, 600 °C and 800 °C for an hour, to evaluate the impact of calcination of structural and catalytic properties. The catalytic tests were performed in a flow reactor, at 150 – 650°C and atmospheric pressure. All the catalysts showed high conversion for CO_2, including the combustion synthesized CeO_2 without any metal loading. The selectivity of the product was found to be highly dependent on the nature of active site, where Cu was selective for CO only and Ni showed selectivity for both CO and CH_4. Both the catalysts showed stable performance for 20h time on stream (TOS) run without showing any decay in conversion. Based on our detailed analysis (XRD, SEM, TEM, XPS) a strong dependence on the reducibility of CeO_2 support was found, which indicates the oxygen defects to be a participating agent in CO_2 conversion chemistry.

Biography:

Anand Kumar is an Associate Professor in the Department of Chemical Engineering at Qatar University. He obtained his Ph.D. in Chemical Engineering (2011) from the University of Notre Dame, USA, and B.Tech. (2006) from IIT Kharagpur, India. His research interests include heterogeneous catalysis, electrocatalysis, hydrogen production, hydrocarbon reforming, and CO_2 conversion.

Catalytic synthesis mechanisms of endohedral carbon nanostructures

Umedjon Khalilov[1,2]*
Kamoliddin Mehmonov[1]
Erik C. Neyts[2]

[1]Institute of Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan
[2]University of Antwerp, Antwerp, Belgium

Abstract

Nanomaterials with controllable dimensions are motivated by the possibility of growing new carbon nanostructures inside carbon nanotubes. However, a full understanding of the mechanisms of the catalytic synthesis of such endohedral carbon nanostructures is still elusive.

In our simulation-based study, we investigate the Ni-catalyzed growth mechanism of endohedral carbon nanostructures from different carbon C_x and hydrocarbon C_xH_y and oxygen-containing hydrocarbon $C_xH_yO_z$ precursors using reactive molecular dynamics simulations and first-principles calculations [1-3]. In particular, our simulation results show that the catalyst-assisting nucleation and consequent growth of different endohedral carbon nanostructures, i.e., nanotube, nanoribbon, carbyne, etc., can be determined by the choice of different carbon-containing feedstocks [1,2]. On the other hand, the results indicate that all obtained nanostructures contain metal (catalyst) atoms, and such structures are less stable than their pure counterparts [1]. Consequently, the oxidation-based purification mechanism of these structures is also studied [1]. Moreover, we find that chemical modification of the obtained endohedral carbon nanostructures results in structural changes and semiconducting to metallic transition [2,3]. Overall, this study opens a possible route to the selective synthesis of encapsulated carbon nanostructures with tunable electronic properties.

Biography:

Umedjon Khalilov is Chief Researcher at the Institute of Ion-Plasma and Laser Technologies (IPLT), Academy of Sciences, Uzbekistan since 2021, and is head of the interdisciplinary research group NanoSim. He obtained his Ph.D. in Chemistry from the University of Antwerp (UA), Belgium in 2013. The work was done in collaboration with IMEC, Belgium. Subsequently, he worked as an FWO fellow (2014-2020 in UA) on molecular dynamics simulations of new carbon nanostructure synthesis. He is currently the Principal Investigator of the fundamental research project in collaboration with IPLT and UA.

Biofunctionalized ZnS Quantum dot/Polypeptide Nanoconjugates with Photocatalytic and Antibacterial Activities for Potential Water Treatment and Disinfection

Alexandra A. P. Mansur[1]
Elaine M.S. Dorneles[2]
Andrey P. Lage[3]
Herman S. Mansur[1]*

1Center of Nanoscience, Nanotechnology, and Innovation – CeNano2
[I] Department of Metallurgical and Materials Engineering, Universidade Federal de Minas GeraisUFMG.
[2] Departamento de Medicina Veterinária, Universidade Federal de Lavras, UFLABrazil;
[3] Departamento de Medicina Veterinária Preventiva, Federal University of Minas Gerais, UFMG, Brazil;

Abstract:

The pollution and contamination of water bodies with a wide-ranging of chemical hazardous and microbiological substances is a theme of raising global environmental concern. Hence, in this work, we developed new nanoconjugates composed of ZnS quantum dots (ZnS-QDs) surface functionalized by epsilon-poly-L-lysine (εPL) (ZnSQD@εPL) synthesized through an eco-friendly and biocompatible aqueous route.

These nanoconjugates were characterized by their physicochemical properties associated with spectroscopic and morphological features. The results demonstrated that chemically stable ZnS-QD@εPL colloidal nanoconjugates were effectively formed with positively surface-charged features due to the cationic nature of the amine-rich polypeptide. Moreover, these nanoconjugates demonstrated photocatalytic degradation of methylene blue (MB) as a model organic dye pollutant combined with moderate antibacterial activity against gram-negative and gram-positive strains. It can be envisioned that these novel nanoconjugates offer innovative nanoplatforms for potential water treatment and disinfection alternatives relying on sustainable materials and processes, preventing negligent discards of organic pollutants and pathogens in water bodies and aquatic ecosystems.

Synthesis of a Novel Spinel Nanocomposite for the Photodegradation Application Under Visible light Illumination

Karim Tanji

Université Sidi Mohammed Ben Abdellah, Morocco

Abstract Not Available!!!

Calculating the adsorption energy of a charged adsorbent in a periodic metallic system – the case of BH4 hydrolysis on the Ag(111) and Au(111) surfaces

Haya Kornweitz1*
Dan Meyerstein1,2
Basil Raju Karimadom1

1 Chemical Science Department and The Radical Research Centre, Ariel University, Israel
2 Chemistry Department, Ben-Gurion University, Beer-Sheva, Israel

Abstract

Many heterogeneously catalyzed reactions involve the adsorption of charged species on metals. DFT calculations of charged systems, with periodic boundaries, face serious problems, concerning convergence and reliability of the results. To study the heterogeneously catalyzed reactions, a simple method to calculate the adsorption energy of charged systems in metallic periodic cells is proposed. In this method, a counter ion is placed at a non-interactive distance, in an aqueous medium, so that the calculated system is neutral. Bader analysis is used to validate that the calculated couple is charged correctly.1This method was used to explore the hydrolysis of BH4 ions, which have a high theoretical hydrogen storage capacity, on the Ag(111) and Au(111) surfaces. It is proposed that the BH4-hydrolysis and reduction mechanisms catalyzed by

M0-NPs depend considerably on the nature of the metal.

Biography:

I am an associate professor in the department of Chemical Sciences in Ariel University, Israel. I am exploring computationally fundamental aspects of reactions e.g., the mechanism of a reaction and the effect of various catalysts (homogenous and heterogenous). I am using mainly DFT methods as implemented in g16 and VASP software.

Antioxidant Nanozymes to Maintain the Redox Environment within Artificial Red Blood Cells

Leticia Hosta-Rigau*
Michelle M. T. Jansman
Xingli Cun
Xiaoli Liu

DTU Health Tech, Center for Nanomedicine and Theranostics, Technical University of Denmark, Denmark

Abstract

Nanozymes are nanoparticulate systems with enzyme-like catalytic properties. Importantly, nanozymes can overcome some of the drawbacks of biological enzymes such as their high production costs, short catalytic half-lives, limited number of active sites and sensitivity to the environmental milieu.

Herein, we present three different nanozymes displaying antioxidant catalytic activity (i.e., cerium oxide (CeO_2) and gold (Au) nanoparticles (NPs) and nanoclusters (NCs)) which have been developed to minimize hemoglobin (Hb) autoxidation. Hb, which is the main component of our red blood cells, has evolved to have excellent oxygen carrying properties and, thus, is currently used to create the so-called Hb-based oxygen carriers (HBOCs). HBOCs are being explored as an "oxygen bridge" to replace blood transfusions in situations where donor blood is not available (e.g., in a life-threatening context such as trauma prior hospital admission or in remote locations or austere battlefield). In contrast to donor blood, HBOCs are compatible with all blood types, thus avoiding the need for cross matching, have unlimited availability are free from infection risks and can be stored for a long time.

However, a prominent challenge when developing HBOCs is the autoxidation of Hb into methemoglobin (metHb) which lacks the ability to deliver oxygen. To address this limitation, we have developed HBOCs incorporating CeO_2-NPs, Au-NPs or Au-NCs. Their catalytic potential is demonstrated in terms of superoxide radical- and peroxide-scavenging abilities which are two prominent reactive oxygen species that exacerbate metHb conversion. This catalytic activity, which is maintained over several rounds, successfully translates into a decreased metHb conversion.

Biography:

Leticia Hosta-Rigau is, since 2015, the leader of a research group which currently consists of 3 postdocs, 4 PhD students and several MSc students. Her research line aims at creating advanced, high-performance materials for therapeutic delivery and regenerative medicine using biologically inspired paradigms. A major direction in this context is the creation of red blood cell mimics to be used in emergency situations where donor blood is

not available. In 2020, she was awarded an ERC Consolidator Grant to pursue this goal. Her H-factor is 34 and has published over 55 papers and attracted ~3.200 citations.

Photo-assisted phenol removal from aqueous solution: a comparison among photo-catalysts

Diana Sannino*
Nicola Morante
Vincenzo Vaiano

Salerno University, Department of Industrial Engineering, Italy

Abstract

Phenols and their derivatives are well known to be biorecalcitrants and for their acute toxicity. Phenol along with its chloro- and nitro-derivatives is highly soluble in water, hence its removal from aqueous solution, despite hardly operated by conventional wastewater treatment, is desired. Photo-assisted processes are able to treat refractory compounds leading to partial or total oxidation also of phenol among them. In particular, photocatalysis and Photo-Fenton process can be exploited for the phenol removal. Intermediates such as hydroquinone, catechol, and p-benzoquinone as major side-product can be individuated during the photocatalytic degradation of phenol. In this work, several photocatalysts are presented, Fe doped TiO_2, Cr-doped TiO_2, co-doped Fe_Cr-TiO_2, prepared by wet chemical methods, and reduced iron-zeolites and proven in phenol photodegradation under solar or visible light irradiation. The influence on the phenol removal of metal loading was also evaluated. The pH also plays a role in the photocatalytic removal of phenol. Further tests assisted by the addition of H_2O_2 as further oxidant, led to high conversion in lower treatment time, namely 2 hours. The results are compared with the literature studies.

Biography:

Sannino obtained MSc in Industrial Chemistry (University of Naples) and PhD in Thermomechanical Engineering Systems (University of Salerno, Italy). Associate professor at Department of Industrial Engineering (Salerno University, Italy) her research interests focused on the heterogeneous catalysis deals with the synthesis and characterization of nano- and structured-catalysts, the coupling with phosphors, as well as mechanism and kinetics of photocatalytic reactions for the removal of pollutants, mild organic syntheses, photoreforming to produce hydrogen, the photoreactor engineering, the energy saving in photocatalysis. She has published more than 180 journal papers (H-index=40) and several Italian and international patents.

Environmental applications of photocatalytic TiO_2 films obtained by anodic oxidation

Maria Vittoria Diamanti*
MariaPia Pedeferri

Politecnico di Milano, Department of Chemistry, Materials and Chemical Engineering “Giulio Natta”, Italy

Abstract

The interest in titanium and its oxides keeps growing on account of their peculiar engineered properties, which find applications in several fields, from architecture to bioengineering, from automotive to photovoltaic cells and photocatalytic devices, as well as to produce self-cleaning

surfaces. There are several methods that allow to grow titanium oxides, among which anodic oxidation has the nice advantage of growing TiO_2 nanostructures directly immobilized on a substrate, avoiding the issue of nanostructure recovery from the medium. The different procedures and parameters of anodic oxidation will be described, giving information on the main oxide characteristics achievable: thickness, morphology, structure and composition. An analysis of the fields of application associated with specific oxide characteristics will be provided.

The experimental data here presented will then focus on latest achievements in the field of environmental cleanup with photocatalytic TiO_2 oxides. Indeed, anodic titanium dioxide is often tested in purification devices, for both wastewater and air treatment: the main goal is to achieve large surface area and high oxide crystallinity, in order to ensure the formation of oxides with high photocatalytic activity. In this direction, the production of self-aligned TiO_2 nanotubes that stem vertically from the metal substrate is the preferred technique, as it allows to achieve specific surface areas even two orders of magnitude larger than the nominal one. Oxides are then tested in the degradation of organic dyes as representative of possible water contaminants, and in the degradation of volatile organic compounds (VOCs).

Biography:

Maria Vittoria Diamanti (PhD in Materials Engineering) is Associate Professor at the Department of Chemistry, Materials and Chemical Engineering "Giulio Natta" of Politecnico di Milano. Her research interests are mostly related to the production, characterization and applications of nanostructured titanium oxides, either grown by electrochemical techniques on titanium and its alloys, or as nanoparticles or sol-gel applied to different substrates as coating or in bulk (polymers, glass, mortars...). She is author of more than 70 articles on international Journals (Scopus h-index 24), editor of 3 books, 2 international Journals and guest editor of 5 special issues of international Journals.

Using Photcatalysts to Achieve Germicidal Action

Mirela Suchea

CEMATEP, School of Engineering, Hellenic Mediterranean University, Greece & IMT-Bucharest, Romania

Abstract Not Available!!!

Biocatalytic Nitro Reduction: From Hit to Process

Amin Bornadel*
Beatriz Domínguez

Johnson Matthey Plc, U.K.

Abstract

Reduction of nitroaromatic compounds is a well-established technique using a range of chemocatalytic techniques. Our recently developed technology involves a biocatalytic approach combining a nitroreductase enzyme and vanadium for an efficient, chemoelective reduction of nitroaromatics to anilines. This technology has been developed in a collaboration between Johnson Matthey and Amgen.

Biography:

Amin Bornadel, Team Leader of the Enzyme Applications Team within the Biotech Group at Johnson Matthey, with PhD in Biotechnology from Lund University in Sweden and MSc in Chemical and Biochemical Engineering from LTU in Sweden.

In Situ Formation of Cationic π-Allylpalladium Precatalysts in Alcoholic Solvents: Application to C–N Bond Formation

Frederic Bihel

University of Strasbourg, France

Abstract Not Available!!!

Activation Tailoring in Few Layer Graphene-Metal Oxide Composites

Izabela Janowska

University of Strasbourg, France

Abstract Not Available!!!

Metal-doped TiO_2 composite nanofibers with improved photocatalytic performance for degradation of organic pollutants

Petronela Pascariu[1,2]*
Mirela Suchea[2,3]

[1]"Petru Poni" Institute of Macromolecular Chemistry, Romania
[2]Center of Materials Technology and Photonics, School of Engineering, Hellenic Mediterranean University (HUM), Greece
[3]National Institute for Research and Development in Microtechnologies (IMT-Bucharest), Romania

Abstract

Nowadays, water pollution caused by industrialization, population growth, and global warming has determined the development of new methods for obtaining clean water. Nanostructured oxide semiconductor materials have been of particular interest due to their potential applications in purification and environmental protection. This presentation summarizes the performance of the metals doped TiO_2 semiconducting materials developed by the electrospinning-calcination method and applied in photocatalytic systems for the degradation of some pollutants. Specific details regarding the synthesis, characterization, application, and mechanism of action of these semiconducting catalysts are highlighted. Moreover, it was proved that the photocatalytic performances of these materials can be improved by doping with different transition metals and lanthanides. The 1D nanostructures were tested as photocatalysts for methylene blue (MB) dye and ciprofloxacin (CIP) drug pollutant degradations under visible light irradiation. The kinetics of MB and CIP photodecomposition reactions were analyzed. The materials showed remarkable photocatalytic activities for optimal photodegradation conditions with rate constants of the order of 10^{-1} min^{-1}. Likewise, TOC removal efficiencies were found to be approximatively 70 % for the mineralization of MB and CIP, respectively, after t = 360 min of reaction time, which are relevant results in the present state of the research. All photocatalysts displayed excellent re-

usability (after 5 cycles of use under identical conditions) for the photodegradation of the two pollutants (MB and CIP).

Biography:

Petronela Pascariu is an experienced researcher at the "Petru Poni" Institute of Macromolecular Chemistry from Iasi, Romania. Her main scientific interests involve the design, synthesis, and investigation of nanoparticles, thin films and multilayers nanowires, metal oxide ceramic nanofibers based on ZnO and TiO_2 doped with various metals, composites, polymer/inorganic nanoparticles nanostructures, with specific optical, electrical, photocatalytic and magnetic properties for use in various modern applications (photocatalysis, sensors, electronics and optoelectronics, electrochemical supercapacitors, etc.). She is a co-author of 60 scientific articles published in ISI-rated international journals (1172 citations), 7 book chapter and more than 95 presentations including areas, such as: nanotechnology, materials science, engineering, physics, chemistry, electrochemistry, etc.

Catalytic functionalization of industrial filter textiles for emission reduction

Andreas Roppertz*[1]
Robert Groten[2]

[1] Department of Chemistry, University of Applied Science Niederrhein, Germany
[2] Department of Textile and Clothing Technology, University of Applied Science Niederrhein,-Germany

Abstract

Catalytic emission reduction for stationary applications such as waste incineration or paint shops is becoming increasingly important. Here, the focus is particularly on simultaneous particle and emission reduction. For this purpose, multi-layer filter bags are usually used, in which the catalytic function is separated from the filter function. We developed a catalyst technology that can be deposited on conventional polyester-based filter textiles without affecting their origin properties. This allows to use a single-layer filter bag for the simultaneous removal of particles and emissions. Such novel catalytic systems can significantly improve the energy efficiency of the exhaust gas cleaning system.

Biography:

Andreas Roppertz is Professor of Technical Chemistry at the University of Applied Science Niederrhein. He has been working in the field of heterogeneous catalysis for emission reduction for more than 10 years. Beside the development of new sustainable catalysts, he also conducts research on bifunctional non-classical catalysts.

Copper catalyzed dearomatization of N-heteroaromatic compounds

Marta Castiñeira Reis[a]
Syuzanna R. Harutyunyan*[b]

[a]Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares, University of Santiago de Compostela, Rúa de Jenaro de la Fuente, CP 15705, Santiago de Compostela, A Coruña, Spain
[b]Stratingh Institute for Chemistry, University of Groningen,

The Netherlands, Nijenborgh 4, 9747 AG Groningen

Abstract:

1,4 Conjugate additions (CA) have been widely exploited in the enantioselective formation of new C-C bonds.[1] However, we are still far from a complete understanding of how they work.[2] With the aim of understanding the mechanism behind the enantioselective CA of Grignard reagents to different aromatic Michael acceptors, we investigated the copper catalyzed addition of EtMgBr to different N-aromatic substrates (pyridine, 2-MeO-pyridne and 4-MeO-pyridine) in the presence of a chiral ligand (**Figure 1**). Our mechanistic investigations have allowed us to identify not only the copper active species but also the nature of the species formed in solution and the process through which chirality is transferred to the product.

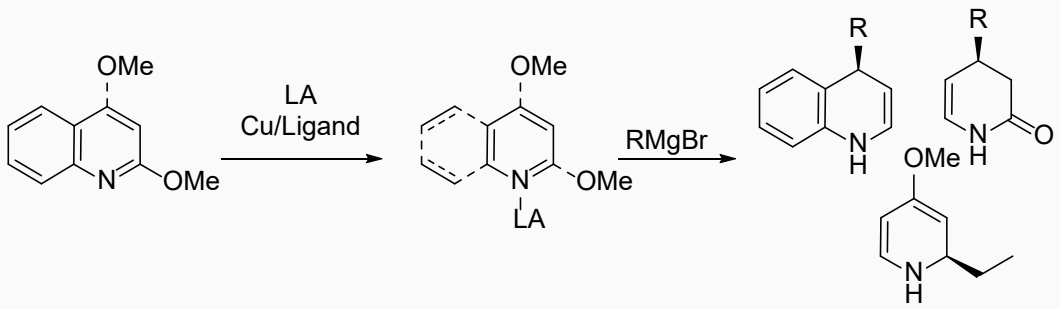


Figure 1.

Biography:

Marta Castiñeira studied Chemistry at the University of Vigo (Spain) from 2007-2012. In this university she also obtained her Master in Advanced Chemistry (2013) and PhD degree (2019). After, she moved to the University of Groningen (The Netherlands) to continue her career as a postdoctoral researcher until April, 2022. Currently, she is a postdoctoral researcher at the University of Santiago de Compostela. Her research interests focus on the mechanistic elucidation of metal catalysed processes and pure organic transformations.

Surface Catalysis for the Self-Assembly of Amyloidogenic Proteins

Yuri Lyubchenko

University of Nebraska Medical Center, Omaha, NE

Abstract Not Available!!!

Keynote Presentations

Potential Drug Development for Epigenetic Enzyme Targets for Cancers

Debbie C. Crans

Colorado State University, Fort Collins, CO

Abstract Not Available!!!

Plastic Trash to Monomers and Intermediates – PTMI

Anne M. Gaffney

University of South Carolina, Columbia, South Carolina, USA

Abstract:

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 down-cycles 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 waste stream. Current high TRL feedstock recycling technologies like pyrolysis and gasification are highly energy intensive, require multiple steps (plastics-syn-gas-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.

Biography

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.

High Oxidation State Arylimido -Alkylidene Complexes with Vanadium and Niobium Complexes as Catalysts for Olefin Metathesis Polymerization

Kotohiro Nomura*

Department of Chemistry, Tokyo Metropolitan University, Hachioji, Japan

Abstract

Certain high oxidation state metal–alkylidene complexes with early transition metals have been known to play essential roles as catalysts in olefin metathesis reactions, which have been recognized as the useful method for synthesis of functional polymers as well as fine chemicals. In contrast to successful examples demonstrated by molybdenum and tungsten [1], the reports by group 5 transition metal-alkylidene complexes still have been limited [2]. In this lecture, we wish to introduce our recent reports for synthesis of vanadium(V)–, niobium(V)–alkylidene complexes-containing both arylimido and halogenated phenoxide or alkoxide ligands, and their use as the olefin metathesis polymerization catalysts [3]. In particular, our efforts for cis specific (living, chain transfer) ring-opening metathesis polymerization (ROMP) of cyclic olefins and living polymerization of internal alkynes will be introduced. More recent results in highly active niobium–alkylidene catalysts for ROMPs and stereospecific synthesis of bottle brush ROMP polymers will also be introduced.

Biography:

Kotohiro Nomura finished his master studies in University of Tokyo, and joined as a research scientist in Sumitomo Chemical Co., Ltd in 1988. He received his Ph.D. in 1993 from Osaka University and joined Massachusetts Institute of Technology as a postdoctoral fellow. He once returned Sumitomo and became an associate professor in Nara Institute of Science and Technology in 1998. Since 2010, he has been a full professor in Tokyo Metropolitan University. He has co-authored more than 350 publications, and his recent research focuses on design of molecular catalysts for efficient carbon-carbon bond formation and chemo-specific organic transformations.

Oral Presentation

Analysis of coumarins as organic photocatalyst used in organic synthesis

Selene Lagunas-Rivera*
Salma Mora-Rodríguez, Miguel A. Vazquez
Marco A. Revilla
Juan Manuel Peralta Hernándeza

Departamento de Química, DCNyE, Universidad de Guanajuato, México.

Abstract

The most important advance in photocatalysis in the last decade has been the synthesis and application of organic compounds used to generate C-C, C-N, C-O, C-S bonds due to the versatility of organic molecules that allows adjusting their photochemical and photophysical properties, their low cost, as well as their high availability. The photochemical properties to consider a

good photocatalyst, such as: absorption wavelength preferably in the visible region, high molar extinction coefficient (ε) and efficiency to go from the singlet state (S1) to the triplet excited state (T1), long lifetimes of the triplet state and high potential redox. Organic dyes have shown ecological and economic advantages over organometallic compounds due the redox potential of the excited state is suitable for the catalysis of many photooxidation and photoreduction reactions formerly promoted by a metal photocatalyst. Also, these dyes exhibit strong absorption in the visible spectrum of light due to their electronic structure. Among these privileged structures are coumarins, which present a wide possibility of functionalizing them through simple reactions, modifying their redox properties, expanding the possibility of being applied to various substrates. However, their use as photocatalysts has been little explored, opening the possibility of analyzing coumarins coupled with amines, and their photocatalytic activity was studied using model reactions.

Biography:

Selene Lagunas-Rivera was born in Mexico City where she studied Chemistry. In 2008 she got his Ph.D in at the Escuela Nacional de Ciencias a Biológicas-IPN working in the field of asymmetric synthesis, by the guidance of Prof. Gerardo Zepeda. Afterwards, she worked as a postdoctoral fellow at the Instituto de Biotecnología-UNAM and the Centro de Investigaciones QuímicasUAEM. Currently, she is a CONACyT-funded lecturer at the University of Guanajuato. Her research interests include the chemistry of natural products and green chemistry applied in photochemistry.

3D-Printed TiO_2NPs Photocatalysts Design: Photodegradation of Air and Water Contaminants.

José Bonilla-Cruz[1,*]
Manuel A. Ávila-López[1]
Tania E. Lara-Ceniceros
Alfredo Aguilar-Elguezabal[3]

[1]Nano & Micro Additive Manufacturing of Polymers and Composite Materials Laboratory "3D LAB", Advanced Functional Materials & Nanotechnology Group, Centro de Investigación en Materiales Avanzados S.C. (CIMAV-Subsede Monterrey), C.P. 66628 Apodaca, Nuvo-León-México.
[2]Centro de Investigación en Materiales Avanzados S.C. (CIMAV-Chihuahua), 31136 Chihuahua, Chihuahua, México

Abstract

A significant challenge in the photocatalysis field is getting self-supporting three-dimensional (3D)-printable photocatalysts that preserve their photocatalytic activity. Herein, we disclose reusable 3D-printable photocatalysts based on binder-free TiO_2 nanoparticles (3DM-TiO_2) under an eco-friendly, affordable, and reliable methodology for the first time. Strong and mechanically stable 3DM-TiO_2 structures (compression strength = 16 MPa) were obtained under soft sintered conditions (~400 °C), exhibiting an anatase/rutile ratio of 85/ 15% by the Rietveld refinement, a mesoporous structure with a surface area (SBET) of 45.2 m2/g, and outstanding photocatalytic activity. 3DM-TiO_2 successfully demonstrated high recyclability and adaptability in the dust-free photodegradation experiments of emerging contaminants in the liquid phase (triclosan, TCS) and gas phase (liquefied petroleum gas, LPG). A TCS mineralization of ~95% was obtained at 6 h of photodegradation. The reusability from the 3DM-TiO_2 was assessed during 12 cycles of TCS degradation, recovering its photocatalytic activity by 100% after reactivation at 400 °C. In the gas phase, the maximum conversion of LPG to CO_2 was 95.3% for n-butane, 93.7% for isobutane, and 52.9% for propane after 15 h of photodegradation. All photodegradation experiments were

fitted to the Langmuir–Hinshelwood kinetic model. We believe that the technology proposed here could trigger applications of nanomaterial-based photocatalysts, replacing the powdered materials to achieve new reactor designs and process configurations on a large scale.

Biography:

Bonilla-Cruz is Chemical Engineer with MSc in Chem. Eng., and PhD. In Polymers. His research lines span the functionalization of Graphene / Graphene Oxide / Nanoparticles and their Incorporation in Polymeric Matrices for Applications in Sensing, Super-Anticorrosive, Supercapacitors, CO2 Capture, Modulation of the Mechanical Properties of Nanocomposites, Coating. 3D-Printing of polymers, nanocomposites and ceramic materials by stereolithography, Direct Ink Writing and its applications in the development of Catalyst, Photocatalyst, Superhydrophobic Surfaces, Oil-Water Separation, Smart Surfaces, etc.

The use of asymmetric catalysis for the de novo synthesis of oligosaccharide:

George A. O'Doherty

Dept. of Chemistry, Northeastern University, USA

Abstract:

Oligosaccharides plays fundamentally important role in the chemistry of life. This can easily be seen in how cellulose and starch are a critical part in the structure of our cells and a source for energy. The complexity of the carbohydrate monomers (i.e.,6 attachment points in a hexose monomer) makes the structural possibilities of carbohydrate oligomers seem endless. The O'Doherty group has had a long-standing effort aimed at the use of asymmetric catalysis for the practical synthesis of carbohydrate from simple achiral commodity chemicals (e.g., dienes and furans). These approaches have been able to address a range of carbohydrate motifs, from monosaccharides to oligosaccharides. Fundamental to this approach is the development of highly efficient routes that transform, via catalysis, inexpensive achiral chemical resources (e.g., 2-acetylfuran) into enantiopure products (e.g., pyranones), which are poised for the conversion into complex carbohydrate oligomeric motifs. Recently, we have found that these approaches have matured to the point where we have developed enantioselective routes to these oligosaccharides in sufficient quantities that are amenable for biomedical investigations. Successful examples of these types of approaches will be presented. {180 words}

Biography:

George A. O'Doherty: Born in Kilkenny Ireland, the son of two organic chemists, he grew into the family business. He received his BS from RPI working with Professor Alan R. Cutler. After earning his Ph.D. with Professor Leo A. Paquette at OSU, he pursued postdoctoral studies with Professor Barry M. Trost and then Anthony G. M. Barrett. His independent career began at University of Minnesota. In 2002, he moved to West Virginia University. He moved again in 2010, to Northeastern University where he remains. His laboratory is interested in the asymmetric synthesis of biological important carbohydrate and natural products. {99 words}

Structural Determinants of Substrate Recognition and Catalysis by Heparan Sulfate Sulfotransferases

Tarsis Ferreira Gesteira[1]
Tainah Dorina Marfori[2]
Jonathan Wolf Mueller
Matteo Calvaresi[2]
Vivien Jane Coulson-Thomas[1]

[1]College of Optometry, University of Houston, Houston, Texas 77004, United States; [2]Dipartimento di Chimica "Giacomo Ciamician", Università di Bologna, Bologna 40126, Italy; [3]Institute of Metabolism and Systems Research, University of Birmingham, Birmingham B15 2TT, U.K.

Abstract

Heparan sulfate (HS) and heparin contain imprinted "sulfation codes", which dictate their diverse physiological and pathological functions. A group of orchestrated biosynthetic enzymes cooperate in polymerizing and modifying HS chains. The biotechnological development of enzymes that can recreate this sulfation pattern on synthetic heparin is challenging, primarily due to the paucity of quantitative data for sulfotransferase enzymes. Herein, we identified critical structural characteristics that determine substrate specificity and shed light on the catalytic mechanism of sugar sulfation of two HS sulfotransferases, 2-O-sulfotransferase (HS2ST) and 6-O-sulfotransferase (HS6ST). Two sets of molecular clamps in HS2ST recognize appropriate substrates; these clamps flank the acceptor binding site on opposite sides. The hexuronic epimers, and not their puckers, have a critical influence on HS2ST selectivity. In contrast, HS6ST recognizes a broader range of substrates. This promiscuity is granted by a conserved tryptophan residue, W210, that positions the acceptor within the active site for catalysis by means of strong electrostatic interactions. Lysines K131 and K132 act in concert with a second tryptophan, W153, shedding water molecules from within the active site, thus providing HS6ST with a binding preference toward 2-O-sulfated substrates. QM/MM calculations provided valuable mechanistic insights into the catalytic process, identifying that the sulfation of both HS2ST and HS6ST follows a SN2-like mechanism. When they are taken together, our findings reveal the molecular basis of how these enzymes recognize different substrates and catalyze sugar sulfation, enabling the generation of enzymes that could create specific heparin epitopes.

Measuring Charge Carrier Energetics and Transport in Photocatalytic Materials with Ultrafast X-ray Spectroscopy

Scott Cushing*

Caltech, USA

Abstract

Transient X-ray and extreme ultraviolet (XUV) spectroscopy use a core level transition to element specifically measure electron and hole energies as a function of time after photoexcitation. Using reflectivity geometries, few to hundreds of nanometer penetration depths can be achieved to isolate critical surface dynamics. Mobile and polaron-limited carrier transport can also be differentiated through the modulation of the X-ray edge. In this talk, we use transient X-ray spectroscopy to investigate several promising materials for photocatalysis while diagnosing their potential issues. This includes a discussion of mid-gap states and band hybridization effects in $ZnSe_{1-x}Te_x$ alloys, attempts to remove excited state polaron formation in various iron oxide compounds, strong electron-phonon coupling in superatomic materials, and the advances in X-ray theory needed to understand these measurements.

Biography:

Scott Cushing is an Assistant Professor at Caltech with a multidisciplinary background spanning Chemistry, Materials Science, and Physics. His research focuses on the creation of new scientific instrumentation that can translate quantum phenomena to practical devices and applications. The Cushing lab is currently pioneering the use of ultrafast x-ray, time-resolved TEM-EELS, and ultrafast entangled photons for a range of microscopy and spectroscopy applications. Scott has been awarded DOE, AFOSR, Rose Hill, Cottrell, and ACS related Early Career awards. Scott holds multiple patents, some of which led to a solar energy company.

Quantum Dots for Photoelectrochemical Water Splitting

Oomman K Varghese

University of Houston, Houston, TX

Abstract Not Available!!!

Photo-assisted CO_2 chemical reduction in capillary reactors

Reyna Natividad[1,*]
Rosaura Peña Calixto[1]
Lourdes Hurtado Alva[2]
Rubi Romero[1]

[1]Chemical Engineering Lab., CCIQS UAEM-UNAM, Universidad Autónoma del Estado de México, Mexico.
[2]Chemical, Industrial and Food Engineering Department, Universidad Iberoamericana Ciudad de México, México.

Abstract

In the context of sustainability, CO_2 conversion to added-value chemicals is of paramount importance. There are different processes to achieve this and one of them is photocatalysis. The aim of this work was to establish the feasibility to conduct the CO_2 conversion in capillary reactors, photo-catalyzed with 4% Cu-TiO_2 and TiO_2 catalysts. This was conducted in a quartz capillary (0.3 cm diameter and 30 cm length) with 0.5 M NaOH solution at 298 K, under Taylor flow regime and with a 254 nm radiation source. This regime consists of liquid-gas segmented flow. The catalysts were synthesized by catalysts were characterized by atomic absorption to establish the actual copper concentration in the catalyst, Transmission Electron Microscopy, N_2 physisorption, X-Ray Diffraction. The reaction was monitored by HPLC and formic acid was identified as one of the main products. The maximum formic acid concentration was 4033 μmol/g_{cat}·h when the reaction was catalyzed by Cu-TiO_2 (1 g/L) at 298 K, using a 0.5 M NaOH solution and a 254 lamp.

Biography:

Reyna Natividad is a professor at Autonomous University of the State of Mexico since 2005. She earned her PhD from The University of Birmingham, UK. Her research interests are multiphase processes that aim to remediate the environment like advanced oxidation processes and CO2 photoreduction. She has published more than 90 papers and has been guest editor of journals like International Journal of Photoenergy and Journal of Chemistry. Her work has been awarded with the Marcos Moshinsky Fellowship (2018) and The Mexico-UK itinerant Chair (2016). At the present she is supervising several PhD and Master's students.

Thermal decomposition mechanism of Meldrum's acid and its derivatives - theoretical thermochemical and kinetic insights for ketenes formation

Pitambar Poude*

Sarah L. Masters**

School of Physical and Chemical Sciences, University of Canterbury, New Zealand

Abstract

The thermal decomposition reaction of Meldrum's acid (MA) to yield ketene has been studied computationally. Methylene ketene, methyl ketene and dimethyl ketene, derived respectively from methylene Meldrum's acid (MeMA), monomethyl Meldrum's acid (MMMA) and dimethyl Meldrum's acid (DMMA) were also studied. Knowledge of the structure and energetic behaviours of these species enables the mechanism of the ecomposition reactions for MA, MeMA, MMMA and DMMA to be further understood. Two key possible mechanisms with their potential energy diagrams are reported. The first is a single-step reaction with a cyclic transition state and the second is a double-step reaction with two transition states. The composite CBS-QB3 method was used to study the thermochemistry and kinetics of all proposed reaction pathways. Under standard temperature and pressure conditions, all reactions were found to be endothermic requiring activation energies (Ea) in the range of 190 to 250 kJ/mol. Thermodynamic parameters for all the reactions involved were calculated and found to be thermodynamically feasible at 298.15 K apart from MeMA.

Biography

I am a PhD student in the department of Process and Chemical Engineering (University of Canterbury). My present project is about the material preparation, characterization and testing it for Redox flow battery. This abstract is taken from my master's degree (thesis). I have done MSc from school of Physical and Chemical Science, University of Canterbury in 2021. I already published one paper on Chem. Phys. Lette. I also proposed this abstract as my next paper. As a student, I have minimum fund to be there so I will welcome If travel fund available from sponsor. Thank you.

Syntheses and Structures of Gallyliron Complexes with Pyridine Ligands and Their Reactions with α, β-Unsaturated Esters

Takako Muraoka

Gunma University, Japan

Abstract Not Available!!!

Design and Synthesis of Metallo Supramolecular Catalysts Functionalized with Lewis Acidic Sites in the Two-Phase Solvent Systems and Analysis of the Interface Between Organic and Aqueous Phases

Shin Aoki

Tokyo University of Science, Japan

Abstract Not Available!!!

Chemical Approaches Toward Understanding Cysteine Glycosidase Catalysis

Akihiro Ishiwata

RIKEN, Japan

Abstract Not Available!!!

Design of Z-scheme photocatalysis for light-to-chemical conversion

Akinobu Nakada*

Kyoto University, Japan

Abstract

Photocatalytic molecular conversion such as water splitting, CO_2 reduction, N_2 fixation, and photoredox catalysis is of great interest from viewpoints of utilization of solar energy and abundant resources making value-added chemicals. Natural photosynthesis converts CO_2 into sugar using water and sunlight via two-step photoexcitation of photosystem I and II, which is the so-called "Z-scheme". Inspired by the natural photosynthesis, artificial Z-scheme has been constructed as a rational strategy by using two-different photocatalysts for reduction (e.g., H_2 evolution and CO_2 reduction) and oxidation reaction (e.g., water oxidation), and a redox mediator to transport electrons between them. To maximize efficiency of the Z-scheme photocatalysis, development of superior photocatalyst that has appropriate light absorption properties, energy levels and catalytic properties for the purpose reaction is crucial. Herein, engineering of layered bismuth oxyhalides are introduced as a potential candidate of "designable" semiconductor photocatalyst for water splitting.[1-4] In addition, a nature-inspired electron transport system will be presented toward constructing efficient Z-scheme photocatalysis.[5]

Biography:

Akinobu Nakada is a Junior Associate Professor at Kyoto University. He received his Ph.D. from Tokyo Institute of Technology in 2017. During 2017–2018, he joined Kyoto University as a Postdoctoral Fellow and a specially-appointed Assistant Professor. After serving as an Assistant Professor at Chuo University from 2019 to 2021, he was promoted to the present position at Kyoto University. From 2020, he concurrently serves as a PRESTO researcher of Japan Science and Technology Agency. His research interests include molecular engineering into photocatalyst materials/systems for light-to-chemical conversion.

Preparation of a Stable CdS Photoanode for CO_2 Reduction under Visible-light Irradiation

Masanobu Higashi*

Research Center for Artificial Photosynthesis (ReCAP), Osaka Metropolitan University, Japan

Abstract

Metal sulfides are promising visible-light photocatalysts for CO_2 reduction. However, available sulfide photocatalysts are limited because of their instability in aqueous solutions under photoirradiation. In this study, we investigated the fabrication of a stable CdS photoanode for CO_2 reduction. The CdS photoanode prepared by the chemical bath deposition method was subjected to N_2 calcination, which significantly affected its stability. Calcination up to 300 °C did not significantly change the surface morphology of the CdS photoanode. In contrast, the CdS electrode calcined at 400 °C had a smoother surface, with lower surface area of the electrode, which consequently reduced the CdS photocorrosion. $K_2Cd[Fe(CN)_6]$ (particle size ~10 nm) was densely formed on the CdS surface via photocorrosion, and it effectively scavenged photogenerated holes in CdS and enabled the oxidation of $[Fe(CN)_6]^{4-}$ to $[Fe(CN)_6]^{3-}$. Thus, we demonstrated stable CO_2 reduction to CO over the CdS photoanode system in an aqueous solution under visible-light irradiation, along with the oxidation of $[Fe(CN)_6]^{4-}$ to $[Fe(CN)_6]^{3-}$.

Enhanced photocatalytic performance of TiO_2 nanotube photocatalyst by anodization

Sujun Guan[1]*
Yun Lu [2]

[1]Toyo University, Japan
[2]Chiba University, Japan

Abstract

Currently, the novel severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) causative agent of the COVID-19, which is a global pandemic, has infected more than 552 million people, and killed more than 6.3 million people. SARS-CoV-2 can be transmitted through airborne route in addition to direct contact and droplet modes, the development of disinfectants that can be applied in working spaces without evacuating people is urgently needed. TiO_2 is well known with some features of the purification, antibacterial/sterilization, making it could be developed disinfectants that can be applied in working spaces without evacuating people.

Facing the severe epidemic, we expect to fully expand the application of our proposed effective approach of anodization, which can be prepared on a large-scale fabrication of an easy-to-use TiO_2/Ti photocatalyst coating, with hope to curb the epidemic.

In this study, TiO_2 nanotube arrays were prepared by anodization. The diameter and length of the TiO_2 nanotubes were measured. The influence of the applied voltage, distance between the electrodes, addition amount of NH_4F on TiO_2 nanotube arrays were discussed. The photocatalytic activity was investigated. The diameter increases with increasing of applied voltage with a liner relationship. The length increases with applied voltage and has an exponential relationship. The moving of the ions and reactions in the anodization were discussed. The TiO_2 nanotube arrays had high photocatalytic activity.

Biography:

Guan is an associate professor working in the Bio-Nano Electric Research Center at Toyo University from April 2021, focusing on visible-NIR-driven photocatalysis and their environmental and bio application. Prior to this, he worked at the Department of Physics at Tokyo University of Science from April 2017, researching on the visible-driven photocatalysis, p-type ZnO semiconductor films and their related devices. Before the work, he gained his PhD in Department of Mechanical Engineering at Chiba University, working on enhancement of visible-light absorption and photocatalytic activity of TiO_2 photocatalyst coatings.

Biocatalytic CO_2 hydrogenation into formic acid by immobilized bacterial cells

Ki-Seok Yoon[1,2,3]*
Mohammad Moniruzzaman[1,2]
Nguyen Khac Hung[1,3]
Kiyasu Yu[1,3]
Seiji Ogo[1,3]

[1]International Institute for Carbon-Neutral Energy Research (WPI-I2CNER), Kyushu University [2]Mitsui Chemicals, Inc.-Carbon Neutral Research Center (MCI-CNRC), Kyushu University [3]Department of Chemistry and Biochemistry, Graduate School of Engineering, Kyushu University, Japan

Abstract

Catalytic reduction of CO_2 to formic acid by using H_2 has received increasing attention because of the growing importance of carbon abatement technologies, hydrogen energy carriers, and carbon-neutral chemical feedstocks. To date, various types of homogeneous and heterogeneous catalysts have been synthesized to develop efficient systems for the catalytic production of formic acid from CO_2 and H_2. Recently, biocatalytic CO_2 hydrogenation has achieved extensive attention, however, traditional enzyme catalysts are limited by issues such as catalytic instability and lower repeatability. In contrast, the whole-cell bio-catalysis has drawn extensive attention, since it not only avoids multistep enzyme extraction and purification, but also preserves inherent optimal conditions for enzyme cascades in bacterial cells. In this study, we developed a highly active and robust system for biocatalytic CO_2 reduction by coupling with H_2 oxidation using the immobilized bacterial cells. The immobilized cells were prepared by encapsulating the grown cells inside hydrogel matrix of gellan gum by cross-linked with calcium ions. The bio-hybrid catalyst efficiently catalyzed the hydrogenation of CO_2 to yield only formate under ambient conditions of H_2 and CO_2 (70:30, v/v%) conditions. The immobilized cells in hydrogels can retain over 90% of its initial activity even after ten repeated cycles, suggesting its great potential for industrial applications.

Biography:

Ki-Seok Yoon received his education and professional training at the University of Tokyo (PhD in 1996), the Ohio State University (postdoc from 1996-2001). After the number of research careers, he was appointed to his current position of a WPI associate professor in Kyushu University at the International Institute Carbon-Neutral Energy Research (WPI-I2CNER) in 2013. His laboratory explores the interface of microbiology, biochemistry, and synthetic chemistry relevant to the development of biological and synthetic catalysts for the sustainable synthesis of fuels and chemicals from small molecules such as hydrogen and carbon dioxide.

α-Functionalization of Carboxylic Acids Driven by Boron Catalyst and Visible Light

Yohei Shimizu[1,2]*
Kai Sun[1]
Masato Ueno[1]
Takuto Morisawa[1]
Tsubasa Oyama[1]

Masaya Sawamura[1,2]

[1]Department of Chemistry, Faculty of Science, Hokkaido University, Japan
[2]Institute for Chemical Reaction Design and Discovery (WPIICReDD), Hokkaido University, Japan

Abstract

Carboxylic acids are ubiquitous motif in biologically active compounds. Although catalytic α-functionalization of carbonyl compounds is a well-studied approach, direct use of carboxylic acid as a substrate is less developed compared to that of other carbonyl compounds. The difficulty mainly stems from the low acidity of α-proton, which hampers the formation of an enolate under catalytic conditions. In this context, a boron-catalyzed enolate formation of carboxylic acids under mild organic base conditions was developed. In situ generated carboxylic acid enolates, the diboron enediolates, reacted with various electrophiles via polar reaction pathways. Herein we extended the method to a radical reaction by combining the boron catalyst with photoirradiation to promote α-allylation of α-arylcarboxylic acids. The reaction between 2-phenylpropionic acid and 2-phenylallylsulfone with a boron catalyst was conducted under blue LED irradiation conditions. Intensive studies led to the optimized conditions, which employed allylmesitylsulfone as a reactant, DBU as a base, $(AcO)_4B_2O$/bis-pyrenol as a boron catalyst, and toluene/THF as solvent. Various carboxylic acids, including naproxen and loxoprofen, and allylsulfones gave the products with α-quaternary carbon centers. Furthermore, several control experiments proved the requirement of blue LED irradiation as well as other reaction components. The combination of the boron catalyst and photoirradiation was extended to direct α-amination of carboxylic acids to procure α-amino acids.

Biography:

Yohei Shimizu received his Ph.D. (2011) from the University of Tokyo under the supervision of Professor Masakatsu Shibasaki and Professor Motomu Kanai. In 2011, he started his academic career in Professor Kanai's group as an assistant professor. During this period, he spent 3 months as a visiting scientist in Professor Mathew J. Gaunt's group, Cambridge University (2012). In 2018, he joined Professor Masaya Sawamura's group in Hokkaido University as a lecturer and was promoted to an associate professor in 2020. He has received several awards, including the Thieme Chemistry Journals Award (2020).

Design of Intercalation Catalysts by Use of Anion-exchangeable Layered Inorganic Hydroxides

Takayoshi HARA[1]*
Nobuyuki ICHIKUNI[1]

[1]Graduate School of Engineering, Chiba University, Japan

Abstract

An ongoing objective in the field of catalyst design is the development of innovative materials in which the architecture of the active centers and the bulk morphology at the angstrom or nanoscale play a critical role in determining the catalytic performance. We have already developed two types of anion exchangers, layered hydroxy double salts (HDSs) and layered rare-earth hydroxides (LRHs), as catalyst materials based on the design idea of "Intercalation Catalysts". The introduction of anionic transition metal hydroxide complexes into the Ni-Zn HDS interlayer can generate monomeric species stabilized by strong electrostatic interactions with the host layer. Furthermore, a function-integrated HDS catalyst system, such as a substrate activator and a catalytically active species, effectively catalyzes the various types of organic transformations

in the liquid phase. Considering our success with the application of the Brønsted basicity of the hydroxide layer, the control of the interlayer spacing is also a key strategy for creating an effective catalytic reaction field. Precise tuning of the basal spacing of layered inorganic hydroxides by use of their anion-exchange ability prompted us to examine whether the general synthetic methodology developed could be extended to HDS and LRH as catalyst materials.

Biography:

Takayoshi Hara is an associate professor at Chiba University. He received his Dr. Eng. from Osaka University in 2006 (Prof. Dr. Kiyotomi KANEDA group). He worked at Chiba University as an assistant professor from 2006 to 2016. His current research mainly focuses on development of functional materials using inorganic ion exchangers.

Rational design of coaxial CdS@ZnO nanowire array and efficient photodegradation of methylene blue

Xiuxiu Dong[1,2]*
Ao Huang[1]
Shun Lu[3]
Qiuxiang Zhu[4]*

[1]Jiangsu University, China
[2]Nantong Huaxin center air conditioner Co., Ltd, China
[3]Chongqing Institute of Green and Intelligent Technology, Chinese Academy of Sciences, China
[4]College of Information and Electronic Engineering, Hunan City University, China

Abstract

Herein, we design to synthesize a novel coaxial CdS@ZnO nanowire array catalyst by magnetron sputtering and hydrothermal method. The optimum photocatalytic composite was obtained by controlling the ratio of CdS and ZnO. Take methylene blue (MB) as the model, CdS@ZnO nanowire array (CdS@ZnO-10) photocatalyst exhibited the high photocatalytic activity, and the highest adsorption and photodegradation rate of MB reached 90.38% in 50 min and 99.13% in 120 min under simulated sunlight illumination. The mechanism of heterojunction interface affecting photocatalytic performance was studied. Therefore, the synthesis strategy used in this investigation may provide new design and controllable construction of coaxial structure for organic dye pollutant degradation.

Biography:

Xiuxiu Dong received her Ph.D. degree in biomedical engineering from Southeast University (SEU) in 2020. Currently, she is working in School of Agricultural Engineering, Jiangsu University as a research assistant. Her research interests include the rational design of functional nanomaterials, photocatalysis and the construction of nanobiosensors (e.g., photoelectrochemical sensor, electrochemical sensor), which are applied in tumor marker detection, food safety analysis, environmental monitoring and so on.

Efficiency of Iron Nickel Bimetallic Catalysts in Chemoselective Hydrogenation of Carbonyl Compounds

Muhammad Sadiq[1,3,]*
Umar Wahab[1]

Zaffar Iqbal[2]
Saima Sadiq[3]
Chang Min Kim[3]
Sher Ali Khan[3]

[1]Department of Chemistry, University of Malakand, Pakistan

[2]Department of Chemistry, Bacha Khan University, Pakistan
[3]Department of Chemistry, Kyungpook National University, South Korea

Abstract

Selective hydrogenation of carbonyl moiety in the presence of olefinic group and other reducible functionality is an industrially important transformation. However, the protocol of green chemistry cannot be forfeited for this formidable challenging transformation. Therefore, iron nickel bimetallic recyclable catalyst (Fe/Ni) was used for base free hydrogenation of carbonyl compound with high activity and chemoselectivity in microwave environment. Microwave irradiation, amount of dopant and pre-treatment of catalyst (Fe/Ni) divert conversion/selectivity toward C=O group as compared to C=C or another reducible moiety. The pyridine adsorption studies revealed that pre-treated catalyst with optimal dopant (Fe) possess more acidic sites as compared to untreated catalyst. Furthermore, the selectivity of bimetallic catalysts towards hydrogenation of carbonyl function group was correlated with Fe content present in the matrix of catalyst using combinatorial approach of theory and experiments.

Biography:

Muhammad Sadiq received his PhD degree with specialization in Physical Chemistry in 2009. He joined Department of Chemistry, University of Malakand as Assistant Professor. Now, he is working as a professor in the same Department. During his career, he worked on diverse funded projects to address challenges across physical chemistry, green and sustainable chemistry, material science and reactor engineering, including hydrogenation/ dehydrogenation of ketone/alcohol in liquid/gas phase, photocatalytic oxidation of alcohols, hydrogen production, utilization of carbon dioxide, and application of novel materials.

Stimuli-induced Organocatalysis in Aqueous Media

Chandan Maity*
Nikita Das

Department of Chemistry, School of Advanced Sciences (SAS), Vellore Institute of Technology (VIT), Vellore, Tamil Nadu, India - 632014

Abstract:

As a class of fascinating molecules, enzymes act as biological catalyst accelerating specific reactions in aqueous environment. Enzymes can modulated their catalytic activity in presence of physicochemical stimuli. Enzyme catalysis and related mechanism are the important source of inspiration for developing artificial biomimetic catalysts. Generally, the artificial catalysis take place with the reaction conditions, which has been chosen at the beginning of the reaction. Hence, the control over the chemical process is absent, which would be required for smart applications. Incorporation of stimuli-responsive features into the catalytic systems could solve this issue[1]. However, most of the artificial chemical reactions takes place in organic solvents, which have toxicity issues. Besides, there are risk factors such as flammability, explosivity. With that respect, water is a safe reaction medium, which is abundant, cheap, and environmental

friendly.

Artificial catalytic reactions in aqueous atmosphere have been studied[2]. However, the reactions in water encounter considerable challenges such as solubility, stability of the compounds[3]. Besides, the control over reaction in aqueous atmosphere remains a challenge. In this talk, I will describe how catalytic activity of an artificial system can be controlled by the application of stimuli in aqueous atmosphere[4]

Biography:

Chandan Maity has received his Ph.D. from Humboldt University of Berlin, Germany. Thereafter, he did his postdoctoral research work in Delft University of Technology, the Netherlands and Technical University of Munich, Germany. Currently he is an Assistant Professor at School of Advanced Sciences (SAS) in Vellore Institute of Technology (VIT), Vellore campus, India. He has received "Start-up Research Grant" from SERB, India in 2020. His research group is interested developing stimuli responsive material in "nature-like" environment using functional organic molecules aiming at catalysis, controlled delivery, and biomedical application.

A comparative Study of Pure Chlorophyll and Other Natural Pigments as Sensitizers for TiO_2 for Their Visible Light Photoactivity

Sukanya Krishnan
Ansaf V Karim
Amritanshu Shriwastav*

Environmental Science and Engineering Department, Indian Institute of Technology Bombay Mumbai-400 076, INDIA

Abstract

The dye-sensitized photocatalyst systems involving various natural pigments, such as chlorophylls, carotenoids, and betalains, have immense potential for developing visible light responsive materials for the wastewater treatment. The natural pigments are non-toxic, easy to extract, and abundant in nature. These pigments can be utilized for surface modification of TiO_2 semiconductor nanoparticles, thereby extending the absorption wavelength range to visible light region. The present study deals with the purification of crude chlorophyll pigment extracted from fresh spinach leaves into chlorophyll-a, chlorophyll-b, and carotenoids via flash column chromatography. The three separated and purified pigments along with freshly extracted crude betalains from beetroot were utilized for the synthesis of individual pigment sensitized TiO_2 catalysts via wetness incipient method and after functionalization with salicylic acid (SA). The cyclic voltammetry analysis was performed to identify the potential sensitizing behavior of individual pigments to TiO_2. The synthesized catalysts were comprehensively characterized with XRD, FTIR, TEM, PL, point of zero charge, and XPS. The stability of these functionalized and sensitized catalysts were examined for Ciprofloxacin degradation for 5 reuse cycles at initial pH = 6, catalyst dose of 0.5 g L^{-1}, and initial concentration of CPX = 10 mg L^{-1} under 2 hrs of blue LED light irradiation. It was observed that chl-a, chl-b, and crude chlorophyll pigment sensitized and functionalized catalysts performance reduction was around 3.11%, 2.23% and 2.56% respectively. Besides, all other catalysts viz. carotene, betalains, and cosensitized pigment sensitized and functionalized TiO_2 performance remained unchanged even after 5 reuse cycle operations.

Biography:

Amritanshu Shriwastav completed his PhD from IIT Kanpur where he worked on Algal-Bacterial Photobioreactors for Nutrient Removal. During his Post-Doctoral research, he worked on various

approaches to optimize the algal biorefinery concept. He further worked on Cr contamination from Chromite Ore Processing Residue (COPR). He is currently serving as Associate Professor at IIT Bombay, where his current research is on sonophotocatalytic oxidation processes for emerging contaminant removal, visible light photocatalysis, and occurrence of microplastics in the environment.

Evaluation of Physical Factors in Occupational Health and Safety in a Learning Environment

Peace Onya Ali

Petroleum Training Institute, Nigeria

Abstract Not Available!!!

Poster Presentations

Pharmacological evaluation of novel copper (II) heterocyclic diazenyl pyridinone

Ahlam Ibrahim Alsulami[1]*
Maram Talal Basha[2]
Khadijah Mohamed Alzaydi[3]

University of Jeddah, College of Science, Department of Chemistry, Saudi Arabia

Abstract

Diazenyl pyridinone derivatives have used as condense electron ligands to combined on the Cu (II) centers. The resultant complexes, as well as the evaluation of their compounds as antitumor agents against MCF-7 human breast adenocarcinoma cell line, are conducted to compare their catalysis activity. The finding results indicate that the copper(II)-based complexes show highly inhibitory activity with avoiding the serve side effects compared with the widely used drug of cisplatin on human breast cancer. Moreover, the quantitative relationship between the chemical structure and biological activity has received considerable attention in recent years as a grateful tool to predict theoretical bioactivity in demanding efforts.

Biography:

Ahlam Alsulami, an assistant professor at the University of Jeddah, Inorganic Polymer labs. The research area interest is focusing on the synthesis and use of the inorganic complexes for an industrial and pharmaceutical application. The professional experience as a lecturer in the University of Jeddah, UJ, earned me strong analytical and assessment skills in the teaching lab courses. With a contribution from the organization of King Abdulaziz University, KAU, I won a qualifying Internship Program to King Abdullah University of Science and Technology, KAUST, as a PhD candidate, December 2014 – 2018. Under the supervision of Nikos Hadjichristidis, Distinguished Professor of Chemical Sciences, I have a broaden-experience course and lab skills. Evaluated and improved quality of the publication in Polymer Chemistry Journal with a publication in polymer Chemistry. In order to meet Saudi Arabia's 2030Vision with applicable research, I am interested to build up my future scientific career as a newly PhD graduate, with resources

needed for international research projects and scientific cooperation.

An approach to the investigation of the electrode-solution interfacial region. Comparison of "molecular" and "collective" effects

Victor G. Mairanovsky*

Scientific Society WiGB, Berlin, Germany

Abstract

An approach to the investigation of the electrode-solution interfacial region is proposed, consis-ting in a combined study of the **molecular reactivity** (I) and **the properties of the medium** (II), with the gradual increase in the distance **L** from the electrode surface into the bulk. The (I) is carried out by a comparative structural analysis of the products of direct electro-lysis vs. electrolysis with homogeneous electro-catalyst, for specially chosen substrates, under increase in the **L** (the method "**near-electrode tomography**", NELTO [1]). The (II), in addition to the classical methods of studying the electrical double layer, involves measurements of the viscosity, of the dielectric constant, etc., using **electrochemical atomic force microscope** EC- AFM –techniques [2]. By comparing the data of the NELTO on changes in „**molecular effects**" **x** = f(**L**) with the changes in "**collective effects**" **X** =F(**L**), the new possibilities arise for establishing the nature of phenomena in the interfacial area.
Along with the effects of reactivity, the data of spectral structural nano-measurements can be used as „**molecular** ".
Some results are given and details of this approach are discussed. Presented in part in [3]

Biography

Victor G. Mairanovsky graduated from M. V. Lomonossov MITKHT (Moscow) 1961, Ph.D. (Institute of Electrochemistry, USSR Academy of Sciences, 1966), Dr. chem (Lomonossov Moscow State University, 1980), professor (1985). Worked at the Union Scientific Research Institute of Vitamins VNIVI (1961 - 1993), senior engineer, junior researcher (1963), head of the Lab. control methods of manufacturing (1969), head of the Lab. of physic-chemical Research (1972- 1993). Field: Analyt. and phys. Chemistry, theoretical and applied electrochemistry. Over 200 scientific publications, 30 copyright certificates, patents. Since 1993 in Germany, co-organizer (1996) and board member of the Scientific Society WiGB at the Jewish Community of Berlin.

Conversion of Biorenewable High Fructose Corn Syrup Feedstocks to HMF

Alfred Hagemeyer[1]*
Vince Murphy[2]
Valery Sokolovskii[1]

[1]Alvacat, USA
[2]Rennovia, Inc., USA

Abstract

The present work relates to acid-catalyzed processes for converting fructose-containing biorenewable feedstocks like HFCS (high fructose corn syrup) to HMF (5-hydroxymethyl furfural). HMF can be upgraded by consecutive reduction to hexanetriol followed by hydrogenolysis to the Nylon monomer hexanediol. For HMF reduction, we have previously reported steady state yields to the intermediate BHMF of 90% over 1000 hours TOS [1-2].

Here we present industrially relevant transformations of HFCS into HMF by chemo-catalytic processes in batch and continuous flow reactors [3]. Since long term catalyst stability under hydrothermal conditions is the most important issue for commercial deployment of liquid phase catalysis, we will primarily discuss catalytic performance data for prolonged times on stream.

Homogeneous (mineral acids) as well as heterogeneous (Lewis and Bronstedt acids) dehydration catalysts in mono- and biphasic solvent systems have been screened in high throughput mode [3].

In particular, 75+mol% HMF has been achieved in a continuous flow reactor with HCl in dioxane/water feeding 10wt% HFCS. Polymeric ion exchange resins produced up to 50mol% HMF in IPA or glyme solvents which effectively prevented catalyst deactivation by fouling. 83mol% HMF yield at 98% fructose conversion has been obtained with HCl in dioxane/water using tetraethyl bromide as co-catalyst [3].

Realizing commercial processes will require progress to create stable, water tolerant catalyst formulations and control of catalyst synthesis and reactions conditions to prevent irreversible catalyst deactivation.

Biography:

Alfred Hagemeyer is self-employed since 2018 and cofounder of the contract research company Alvacat offering custom catalyst development for industrial clients. Before starting up Alvacat, he worked for Rennovia from 2011 to 2018 to apply high throughput methodologies to the discovery of catalysts for the production of chemicals from bio-renewable feedstocks. Before joining Rennovia, Alfred worked for Sud-Chemie (now Clariant) from 2006 to 2011, and for Symyx Technologies from 1998 to 2006. Before moving to Symyx, Alfred worked for Hoechst and for BASF, after a Postdoc in Bologna, Italy. Alfred has a Ph.D. in Chemistry from the Max-Planck-Institute in Mainz, a M.Sc. in Physics and a M.Sc. in Chemistry from the University of Dortmund and authored more than 100 issued patents and scientific articles.

Metal supported Activated carbon monolith catalysts from brown coal for Environmental Applications.

Fatima Shahid[1]*
Alan L. Chaffee[1]

[1]School of Chemistry, Monash University, Clayton, VIC 3800, Australia

Abstract

Due to increasing concerns about environmental pollutants, diverse porous materials have been considered for environmental applications, however the most appropriate pore structure and surface functionality, both significant factors for effective adsorption, require determination. Active carbons, in a novel monolithic form, have been prepared from Victorian brown coal (VBC) and are being evaluated for their potential in environmental applications. These monoliths can be modified to provide the selectivity that is required. Iron based heterogeneous Fenton catalysts have been widely employed for degrading organic pollutants, however it is challenging to use them in highly efficient and recyclable application in wastewater treatment. Our synthetic method, produces a novel highly magnetic iron doped carbon catalyst using Victorian Brown Coal (VBC) as carbon precursor. In this work, we have shown that iron-carbon composites prepared from brown coal, via a novel approach, exhibit exceptional activity for the Fenton-like catalytic oxidation of organic matter in water. It is found that some of their tailorable features,

such as large specific surface area, controlled porosity and well dispersed active sites, can effectively enrich organics at low concentrations, thus, facilitating their high efficiency towards degradation of organic pollutants. Results indicate that these iron doped carbon monolith catalysts show the removal efficiency of phenol as high as 98.8% after 5 catalytic cycles and can be used as effective, affordable, and regenerable materials for degrading organic pollutants.

Biography:

Fatima is a PhD student in the Chemistry Department at Monash University. Her research focusses on systematic study of active carbon honeycomb monoliths to explore these materials for a range of adsorbent and catalytic application of prospective environmental benefit.

Ammonia synthesis from H_2O and N_2 using Ru catalysts and electrochemical cells with phosphate electrolytes

Jun Kubota*
Rika Hayashi

Fukuoka University, Japan

Abstract

Ammonia is now synthesized from fossil resources and widely used for artificial fertilizers, so that the infrastructures for transportation and storage has been already available. Ammonia is expected to be carbon-free fuels if it is obtained from nitrogen and water using renewable electricity. The Renewable ammonia can be practically synthesized from a combination of water electrolysis to form hydrogen with renewable electricity and Haber-Bosch ammonia process. However, this combination seems not suitable to fluctuating distributed power sources such as solar and wind plants. We have proposed new ammonia synthesis system which has a Ru-based ammonia catalyst, Pd alloy hydrogen permeable membrane cathode, CsH_2PO_4/SiP_2O_7 electrolyte, and Pt/Ti anode. This electrochemical cell can directly synthesize ammonia from nitrogen and water at 250°C. In this presentation, we are going to explain current progress of the present ammonia synthesis in our group.

The ammonia synthesis cell was operated at 1.0 MPa of absolute pressure and 250°C, and ammonia formation rate of 11.1×10^{-9} mol s^{-1} cm^{-2} was obtained with 6.7 cm^3STP min^{-1} flow of nitrogen at 20 mA cm^{-2}. The current efficiency for ammonia synthesis was estimated to be 16% and 79% of current efficiency was derived for hydrogen production. With increasing current density over 30 mA cm^{-2}, the cell voltage was also increased above 3 V. We examined the overpotentials of cathode and anode using a hydrogen referential electrode. The overpotential of anode was relatively more significant than cathode and the development of efficient anode was found to be required.

Biography

Jun Kubota got PhD of science at Tokyo Institute of Technology in 1995. He was an assistant professor of Tokyo Institute of Technology from 1995 to 2007. His research was study of adsorbed molecules on catalysts using infrared and pulsed laser spectroscopy. He was an associate professor of The University of Tokyo from 2007 to 2015 and started to study photocatalysis and electrocatalysis. He was promoted to a full professor of Fukuoka University in 2015. The current

research interests are electrochemical and catalytic ammonia synthesis from N_2 and H_2O and methane synthesis from CO_2 and H_2O, which are energy conversion from electricity to chemical fuels.

Oral Presentations

Hydrodeoxygenation of esters over bifunctional transition metal phosphide catalysts

Ivan Shamanaev[1]*
Galina Bukhtiyarova[1]

[1]Boreskov Institute of Catalysis, Russia

Abstract:

Transition metal phosphides (such as Ni_2P, MoP) have attracted great interest as promising catalysts for hydrodeoxygenation (HDO) of fatty acid-based feedstocks to produce renewable fuels. Supported nickel phosphides (Ni_2P/SiO_2, Ni_2P/Al_2O_3) outperform sulfide catalysts ($NiMoS/Al_2O_3$ and $CoMoS/Al_2O_3$). However, to obtain active supported phosphide catalysts, great attention must be paid to the methods and conditions of their synthesis.

Study of methyl palmitate (MP – $C_{15}H_{31}COOCH_3$) HDO showed correlation between the amount of acid sites and catalytic activity of Ni_2P/SiO_2 and Ni_2P/Al_2O_3. The acidity of the samples can be varied by the initial Ni/P molar ratio, nature of P precursor, reduction temperature, and nature of the support. A synergetic effect of Ni_2P/SiO_2 and Al_2O_3 mechanical mixture was found [1] and it was concluded that first stage of the process – MP transformation to palmitic acid – is the slowest stage. Increasing in acidity favors acceleration of this stage leading to increasing in overall HDO activity.

HDO has two major routes: direct HDO and decarbonylation/decarboxylation ($DeCO_x$). Direct HDO of MP results in C_{16} hydrocarbons and $DeCO_x$ – in C_{15} hydrocarbons. MoP/SiO_2 is very selective towards the direct HDO (>95%). Similar experiments of MoP/SiO_2 and Al_2O_3 mechanical mixture as well as mixtures with zeolites showed increasing in activity compared to MoP/SiO_2 with inert diluter (SiC) [2].

Finally, the Ni phosphide catalysts were supported on SAPO-11 for HDO-hydroisomerization. The acidity and surface area of Ni_2P/SAPO-11 as well as activity drastically change depending on Ni/P ratio and Ni content, and have completely different tendencies compared to Ni_2P/SiO_2.

Biography:

Ivan Shamanaev is a researcher in Boreskov Institute of Catalysis, working on projects related to phosphide catalysts for hydrodeoxygenation and hydroprocessing reactions. He received his specialist degree in 2014 from the Novosibirsk State University and PhD in 2018 from Boreskov Institute of Catalysis.

Galina Bukhtiyarova completed her PhD at Boreskov Institute of Catalysis. Since 2005 she has been leading a laboratory of hydroprocessing in Boreskov Institute of Catalysis. Her research interests lie in the study of sulfide and phosphide catalysts for hydroprocessing of fossil and renewable sources.

Molecular modeling of promotion effects in cobalt catalyzed Fischer-Tropsch Synthesis

Ali Can Kizilkaya

Izmir Institute of Technology, Turkey

Abstract:

Optimizing product selectivities in the Fischer-Tropsch Synthesis (FTS) has industrial importance due to formation of various products with varying economic values. Although promoters can be useful for this aim, understanding their mechanism towards various products is a challenging task. In this study, Density Functional Theory (DFT) modeling is applied to compare oxidic promoters (in particular praseodymium and sodium) on fcc-cobalt surfaces in FTS with respect to their performances towards selectivity of different products. In accordance with experimentally determined structures, promoted fcc-cobalt nanoparticles are modeled as a combination of flat and stepped surfaces, with oxidic promoter units (PrO_2 and Na_2O) dispersed on them.

Our results indicate that both promoters result induce a significant increase in CO adsorption energy, while the binding strength of atomic hydrogen is slightly reduced. The presence of PrO_2 promoters also leads to a major reduction in the adsorption energy of ethylene. Overall, these results offer insights into how PrO_2 and Na_2O promoters result in increased selectivity to olefinic products. Furthermore, analysis of electronic charge distribution on promoted cobalt surfaces reveals that while PrO_2 species act as electron withdrawing groups, Na_2O species act as strongly electron donating species. These findings compliment the recent experimental findings related to promotion effects on cobalt catalyzed FTS, while providing mechanistic insights related to tuning product selectivity by different promoters[1].

Biography:

Ali Can Kizilkaya obtained his PhD from Eindhoven University of Technology in The Netherlands, related to physical chemistry of catalyst surfaces, combining experimental surface science with molecular modeling. He has worked on the fundamentals of catalytic phenomena such as deactivation and promoter effects on catalyst surfaces, for automotive exhaust catalysis and Fischer-Tropsch Synthesis. After working in industrial R&D in Shell and AkzoNobel laboratories, he currently works on sustainable energy technologies focusing on molecular modeling of heterogeneous catalysts, leading the Kizilkaya Research Lab, in Izmir Institute of Technology in Turkey.

Castor Oil-Based Polyurethane Foam Infused with Modified Diatomaceous Earth for the Removal of Crude Oil

Helanka J. Perera[1]*
Anjali Goyal[2]
Saeed M. Alhassan[3]

[1]Maths and Natural Science, Abu Dhabi Women's Campus, Higher Colleges of Technology, Abu Dhabi, United Arab Emirates
2Department of Chemical Engineering, Khalifa University, PO Box 127788, Abu Dhabi, United Arab Emirates

Abstract:

Hydrophobic foamy materials are of great interest as promising absorbers for the purification of water bodies containing crude oil. We report the synthesis of modified diatomaceous earth particles based on polyurethane foam. The surface of diatomaceous earth particles was modified with octadecyltrichlorosilane to achieve hydrophobicity and lipophilicity. The resulting foam re-

tained a porous structure connected at 130 ° and 85 ° water contact angles on octadecyltrichlorosilane modified diatomaceous earth polyurethane (PU-C18DE) and polyurethane form (PU). Spectroscopic and microscopic analysis was performed to investigate the structure and morphology of PU-C18DE and PU foam. Crude oil sorption tests have shown that PU-C18DE foam is an excellent oil adsorbent with a sorption capacity of 1.31 of its own mass. Therefore, PU-C18DE foam is expected to be a promising oil adsorbent for potential oil spill purification applications.

Biography:

Helanka J. Perera completed her PhD from Oklahoma State University, OK, USA and is currently an Chemistry Assistant Professor in Maths and Natural Science Department at Abu Dhabi Women's College, UAE. Her research interests are in material science, surface modification on micro and nano materials, superhydrophobicity, hydrophobicity, polymer and surface characterization.

Flexible and Stretchable Corrugated Monocrystalline Silicon Solar Cells

Nazek El-Atab

King Abdullah University of Science and Technology, Saudi Arabia

Abstract Not Available!!!

Effect of TiO2 – rgo Nanocomposite in Dye Sensitized Solar Cells

Jasper Ejovwokoghene Ikpesu

University of the Witwatersrand, South Africa

Abstract Not Available!!!

Hight xylitol yield from fresh corncob: an optimized one-pot approach

Yaimé Delgado-Arcaño[1,2]*
Oscar Daniel Valmaña-García[1,2]
Dalmo Mandelli[3]
Wagner Alves Carvalho[3]
Luiz Antônio Magalhães Pontes[4]

[1] University of Guayaquil, Ecuador
[2] Center of Studies for Sustainable Development, ECOTEC Technological University, Ecuador
[3] Federal University of ABC (UFABC), Brazil
[4] Federal University of Bahia (UFBA), Brazil

Abstract:

Xylitol is one of the platform molecules with a high value-added that can be obtained from the xylose contained in biomass. The xylitol production by the chemical route through consecutive reactions in a single reactor is one of the current scientific challenges. In this context, the present work aimed to increase the xylitol yield from fresh corncob through a one-pot approach. For this, an experimental strategy was carried out in two stages. First, to optimize the acid

hydrolysis of the corncob to obtain xylose and subsequently the catalytic hydrogenation of pure xylose to obtain xylitol, using a multifactorial experimental design associated with the response surface methodology; second, to evaluate the hydrolysis and catalytic hydrogenation of the corncob in a single step to obtain xylitol, using the results of the first stage. The xylose yield achieved was 92% ± 1.5% by optimized acid hydrolysis at 140 °C, 1.3% (v/v) H_2SO_4, and 5 min of reaction. A yield of 98 ± 2.5% xylitol was achieved at 140 °C, 2 MPa, 0.1 g of commercial catalyst 5% (w/w) Ru/C, 600 rpm, and 3 hours. By one-pot, fresh corncob was selectively transformed into xylitol, with 71 ± 3.3 yield, at 0.5% (v/v) H_2SO_4, 140 °C, 2 MPa, 1:100 solid/liquid ratio, and 1:5 catalyst/substrate. These results demonstrate that the one-pot strategy, on a laboratory scale, allows obtaining a high yield of xylitol under mild reaction conditions from fresh corncob; and opens perspectives for reducing its production costs and implementing the new process in a biorefinery.

Biography:

I am a Chemical Engineer from the Technological University of Havana, Cuba (2010), a master's degree in Renewable Energy from Jaen University, Spain (2013), and a Ph.D. in Chemical Engineering, from the Federal University of Bahia (UFBA), Brazil (2020). I belong to the research group Catalysis and Environment at UFBA, conducting studies on catalysts and their applications in the use of agro-industrial waste to produce high-added value chemical compounds, and exploring more energy-efficient conversion technologies. I collaborate in the research group on Catalysis and Organic Synthesis at UFABC, Sao Paulo. Currently, I work as a Professor at Guayaquil University, Ecuador.

Metal Oxides Nanoparticles and Nanocomposites for Ammonium Removal from Water

Thamer Adnan Abdullah[a]
Tatjána Juzsakova[b]
Zainab J. Abdel-Zahra[a]
Rashed T. Rasheed[a]

[a] Chemistry Branch, Applied Sciences Department, University of Technology, 19006 Baghdad, Iraq
[s] SustainabilitySolutions Research Lab, University of Pannonia, 8200 Veszprém, Hungary;, Iraq

Abstract:

Rapid increase in the population resulted in industrialization to cope with the needs of bigger population. This industrialization resulted in the environmental pollution which is a threat for the survival of living organisms. Two metal nanoparticles were prepared to remove ammonium from the environment. Cerium dioxide (CeO_2) and vanadium pentoxide (V_2O_5) nanoparticles were prepared by using autoclave method and hydrothermal method, respectively. The removal efficiency of nanoparticles was examined at 90°C and 400°C. The structure, surface roughness, imaging surface and functional group vibrations of these metal nanoparticles were characterized by metal X-ray diffraction (XRD), scanning electron microscopy (SEM), atomic force microscopy (AFM) and fourier transform infrared spectroscopy (FT-IR), respectively. Vanadium pentoxide showed higher ammonium removal efficiency of 70.60% and Cerium dioxide (CeO_2) showed removal efficiency of 40.93% at 400°C. In both cases, removal efficiency was higher at 400°C than at 90°C.

Biography:

Thamer Adnan Abdullah completed his Master of Chemical Engineering from Guru Gobined Singh Indraprastha University New Delhi., in 2012. He is working as an assistant lecturer at the University of Technology, Baghdad, in the Applied Science Department, Chemistry Branch. He completed his Ph.D. from Sustainability Solutions Research Lab, Faculty of Engineering, University of Pannonia, Veszprem, Hungary. He has many articles published in ScienceDirect reputed journals and has participated in many international conferences in the field of Nano-chemistry and Nano-research.

DFT Towards Predictive Catalysis

Albert Poater*
Sílvia Escayola
Michele Tomasini
Anna Vidal-López
Nicolas Joly
Artur Brotons
Roger Monreal-Corona

Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, c/ Mª Aurèlia Capmany 69, 17003 Girona, Catalonia, Spain

Abstract:

With the euphoria for machine learning, there is a branch that goes more unnoticed, predictive catalysis. Thus, what can we do from computational chemistry for sustainability? In the line of machine learning, apply predictive catalysis to the maximum. Thus, on a small scale, the research group tries not only to find the reaction mechanism, and once the rate determining step (rds) is discerned, to look for alternatives to the existing catalysts to reach milder conditions. In detail, this computational research may include from olefin metathesis by Ru-based catalysts or gold chemistry to undertake organometallic reactions to green chemistry to remove and/or not generate CO2: either by water oxidation catalysis or alcohol transformation to aldehydes with generation of H2 as energy source. The mechanisms for the formation of N-substituted hydrazones by coupling of alcohols and hydrazine, achieved by the sequential processes of acceptorless dehydrogenation and borrowing hydrogen,[1,2] has been unveiled by DFT calculations. The release of water and H2 as subproducts, combined with the Mn-PNN pincer based catalyst describe a green environment.[3] Predictive catalysis plays the role to push forward this reaction toward milder conditions, and thus in line with green chemistry standards.

Biography:

Albert Poater (1979) finished the PhD in Chemistry in 2006 at the University of Girona. After periods in Chile with Alejandro Toro-Labbé; in Montpellier with Odile Eisenstein and a long postdoc in University of Salerno with Luig Cavallo, in 2010 he became a Research Scientist in Girona, apart from Visiting Researcher at KAUST-Saudi Arabia, and at LCC-CNRSFrance. In 2019 he became Associate Professor and Head of the Chemistry Department. As a whole, he has published over 250 papers and 10000 citations (H=58), serving as Editor Board of several journals; and in 2019 he received the ICREA Academia Award.

Ni/La-doped CeO_2 catalysts for CO_2 reduction by the reverse water gas shift reaction

Belén Bachiller-Baeza[1]
Maricarmen Capel-Sanchez[1]
Victoria E. García-Sanchez[1]
Joao E. Rodriguez[2]
Javier Gainza[3]
Virginia Perez-Dieste[4]
Carlo Marini[4]
M. Teresa Fernández-Diaz[5]
José A. Alonso[3]
Consuelo Alvarez-Galvan[1]*

1. Instituto de Catálisis y Petroleoquímica (CSIC), Cantoblanco, 28049 Madrid, Spain

2. ESRF (European Synchrotron Radiation Facility), 71 Av. des Martyrs (38000) Grenoble, France

3. Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco, 28049 Madrid, Spain

4. ALBA Synchrotron, Carrer de la Llum No. 2-26, Cerdanyola del Vallès, 08290 Barcelona, Spain

5. Institut Laue Langevin ILL, BP 156X, F-38042 Grenoble, France

Abstract:

The conversion of CO_2 into bulk chemicals and fuels is a process in two steps. The first and essential stage is the reduction of CO_2 to CO with H_2, or reverse water gas shift reaction (rWGS: $CO_2 + H_2 \rightleftarrows CO + H_2O$), using green H_2. The use of an efficient catalyst under the harsh conditions needed is imperative. Several studies suggest that the active site is related to the interface between metallic particles (that activate the dissociation of H_2) and a reducible oxide support such as ceria, with oxygen vacancies that promote the adsorption of CO_2. Oxygen vacancies can be increased by doping ceria with rare earths. The investigation of the oxidation states evolution of metal and support is a key piece for understanding the reaction mechanism. To unravel the role of the active phases, it is essential to approach real conditions and characterize the catalyst under reaction.

In this work, $Ni_{0.1}/(Ce_{1-x}La_xO_{2-x/2})_{0.9}$ catalysts were synthesized (sol-gel method), ex-situ characterized (XRD, TPR, SEM, TEM, N_2 adsorption-desorption, neutron diffraction) and studied in the RWGS reaction. Real-time changes in the local structure and oxidation states of these catalysts during the catalytic reduction of CO_2 into CO were examined via X-ray absorption spectroscopy and over the catalytic surface, by near ambient pressure-XPS. Obtained results revealed that La loading tailors the proportion of Ce^{3+}, producing a direct impact on the reactivity towards the RWGS reaction.

Biography:

Consuelo Alvarez-Galvan completed PhD in heterogeneous catalysts for pentane hydroisomerization, ULL, Tenerife (2000). In 2001, I move to the Catalysis and Petrochemistry Institute (Madrid). My scientific career has been focused on the development of materials and catalysts for different processes of chemical industry, related with energy and environmental protection sectors (removal of volatile organic compounds , hydrogen production and syngas production by hydrocarbon reforming, C1 oxygenates production by direct methane partial oxidation, synthesis of renewable diesel by hydrotreatment of waste oils, RWGS reaction, synthesis and

characterization of inorganic and hybrid perovskites as absorbers in solar cells, among others).

Wood fractionation into valuable molecules in a plug flow reactor using hydrogen free SC alcohols flow and heterogeneous Cu/acid-base catalysts: impact of the alcohols' alkyl chain length

Nadine Essayem[1]*
Awalah A.Komena[1]
Marion Eternot[1]

[1]IRCELYON-CNRS-Lyon1 university, France

Abstract:

In the late 1970s, the use supercritical fluids (SC) in the processing of lignocellulosic biomass appeared in the literature. SC fluids offer possibilities for the liquefaction of lignocellulosic biomass into bio-oils or even directly into chemicals. Here we report the advantages of continuous wood fractionation in a plug flow reactor to face the issues of selective wood biopolymer conversion and its catalytic conversion into valuable molecules, using hydrogen free SC alcoholic solvents and Cu/acid-base catalysts. This implementation presents more advantages than the batch reactor. The possibility of fine tune parameters such the composition of flowing SC organic fluid in addition to T, P presents a high potential in terms of selective and sequential wood fractionation. Conditions for the selective liquefaction of solely lignin without hemicellulose conversion was obtained via the screening of alcohols of variable alkyl chain length up to the corresponding alkane. This result pave the way towards selective and sequential liquefaction of wood biopolymers into valuable molecules, which starts with lignin conversion, then hemicellulose and cellulose. The study of respective solid beds positioning of biomass and solid Cu/acid-base catalysts, leads to molecules yields comparable to the best ones reported in the literature but in hydrogen free conditions

Biography:

Nadine ESSAYEM, Research Director at CNRS at the Institute de Research on Catalysis and Environment of Lyon (IRCELYON) has a recognized expertise in heterogeneous catalysis by solid acids and bases and their applications to Lignocellulosic Biomass (LCB) valorization: from simple C6/C5 sugar or their furanic derivatives transformations to native or isolated cellulose valorization, She acquired expertise on a broad variety of biomass via the coordination of public (national/international) or private collaborations. She is co-author of more than 100 publications in international journals and she filed 21 patents, most of them applied to catalytic biomass valorization.

Understanding the deactivation phenomenon of Ni supported catalysts

José Valecillos*
Leire Landa
Sergio Iglesias-Vázquez
Aingeru Remiro
Ana G. Gayubo

University of the Basque Country UPV/EHU, Spain

Abstract:

The challenges of selecting or designing catalysts comprise meeting an optimum relationship among high activity, selectivity and stability. In many hydrocarbon conversion processes, finding a stable catalyst is indeed a challenge due to the inherent and inevitable formation of carbon (coke) that remains deposited on the catalyst surface blocking the access to active sites or even modifying them causing deactivation. One example is the steam reforming (SR) of bio-oxygenates (e.g. bio-ethanol or bio-ethanol obtainable from biomass) over Ni supported catalysts to produce hydrogen with application in the petrochemical and energy industries. The use of a simple and reproducible Ni/Al_2O_3 catalyst derived from $NiAl_2O_4$ spinel is a promising alternative for the development of this process. Although this catalyst undergoes deactivation by coke, it may be regenerated under appropriate conditions.

For a clear understanding of the catalyst deactivation phenomenon, it is paramount to combine several material surface characterization methods (temperature-programmed techniques, thermogravimetry, spectroscopies and microscopies). It is even more important to make a correct result interpretation from each technique considering their limits of what can and cannot be detected. For example, temperature-programmed oxidation provides the coke quantification and combustion performance with ambiguous information on the nature and location. The use of scanning electron microscopy aids in unveiling the coke morphology and location on the catalyst particle, but this information is limited to the external surface. This lecture addresses these perspectives and challenges based on the experience of studying the deactivation phenomenon of Ni/Al_2O_3 catalysts in the SR of bio-oxygenates.

Biography:

José Valecillos is a researcher at the Catalytic Processes and Waste Valorization group in the University of the Basque Country (Spain). His research focuses on the hydrogen production from biomass derivatives via catalytic steam reforming, particularly studying the catalyst deactivation phenomenon. His prospective research comprises the use of membrane reactors to optimize hydrogen production. He is a bachelor of Chemical Engineering from University of Zulia (Venezuela, 2005) with master's (2009) and doctoral (2019) degrees from University of the Basque Country. His dissertation studied the deactivation of zeolite catalysts in the methanol conversion into hydrocarbons. He has more than 20 publications.

Colloidal synthesis of hybrids graphene-Mo_2C with potential application in water splitting

Daniel Fernández-González [1*]
Juan Piñuela-Noval [1]
Marta Suárez [1]
Adolfo Fernández [1]

[1] Nanomaterials and Nanotechnology Research Center (CINN-CSIC), Universidad de Oviedo (UO), Principado de Asturias (PA), Avda. de la Vega, 4-6, 33940, El Entrego, Spain

Abstract:

Graphene is a carbon allotrope that is formed by a single layer of carbon atoms, which are tightly bounded in a hexagonal honeycomb lattice. It was isolated for the first time by Andre K. Geim and Konstantin Novoselov of the University of Manchester in the early 2000s. From that moment, this material has gained enormous interest due to its promising properties for different

applications. These include high thermal and electrical conductivities, high elasticity and flexibility, high resistance, or antibacterial effect, among other. However, graphene can be decorated with metals, organics, or other phases to improve its characteristics for certain applications, for instance in sensors or catalyzers for water splitting. As it is possible to check, one of the fields where the hybrids graphene-metal phase (i. e. strontium titanate or molybdenum disulfide) is gaining interest is in the field of catalyzers to produce hydrogen from the water splitting. Apart from the above-mentioned combinations, one of the options that is more hopeful in the field of catalyzers for hydrogen evolution is the decoration of graphene with molybdenum (II) carbide. Different alternative methods have been proposed for the synthesis of these nanocomposites, although the common issue of the processes is the complexity of the method with the use of several stages, long processes, or complex reagents. Therefore, a novel process based on colloidal processing method is proposed to synthesize the hybrids using molybdenum chloride as precursor of the carbide.

Biography:

Daniel Fernández González has a Ph. D. in materials, and he is now postdoctoral researcher in the Nanomaterials and Nanotechnology Research Center (which belongs to the Spanish National Research Council). He is author of more than 30 articles and 6 book in the field of synthesis of materials using novel processing techniques as solar energy, spark plasma sintering or laser. He is now working in the field of materials for energy management, including the extraction of manganese sulphate monohydrate from industrial wastes, the synthesis of graphite metal composites for heat sinks or batteries.

Analysis of Charge Distributions in Functional Transition-Metal Tellurides

Priv.-Doz. Dr. Simon Steinberg

Institute of Inorganic Chemistry, RWTH Aachen University, D-52074 Aachen, Germany

Abstract:

Understanding the distributions of atomic charges in materials is decisive for the design of their properties, because many phenomena are linked to these measurable quantum expectation values.[1] In this connection, a new tool has recently been established to extract atomic charges from the results of plane-wave-based computations.[2] In order to understand the charge distributions in transition-metal-containing tellurides which included minerals, ion conductors as well as thermoelectrics, this newly developed population analysis tool has been[3]–[5] applied to these materials, and the outcome of these explorations will be presented in this contribution.

Biography:

Simon Steinberg (∗1987) studied chemistry at the University of Cologne (Germany) where he obtained his diploma in 2010 and his doctorate in 2013. After postdoctoral research stays at Iowa State University/AmesLab and RWTH Aachen University, he started his research as an independent group leader in October 2016 at RWTH Aachen University, where he also completed his habilitation in February 2022. His research interests focus on solid-state and quantum-chemistry with particular consideration of (transition-metal-containing) tellurides.

Impact of the strength of Pd-perovskite interaction in Natural Gas Vehicle three-way catalysts: A kinetic approach

Yuanshuang Zheng, [1]
Pascal Granger[1*]

Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide, F-59000 Lille, France

Abstract:

Natural gas fuelled engines are an alternative to gasoline and diesel engines less pollutant with emission particulate almost nil and lower greenhouse gas and NO_x emissions. However, the complete removal of residual traces of methane, acting as greenhouse gas, remains an important challenge. The complete removal of CH_4 induces the installation of palladium Three-Way-Catalyst (TWC) running at higher temperature to activate methane. To compensate this drawback, highly loaded palladium catalysts can be developed.

Nowadays, an important issue lies in the reduction of critical materials of strategic importance in postcombustion catalysis. The concept of self-regenerative behavior, earlier developed for noble metal-doped perovskite TWC, contributed to enhance conversion at lower temperature and improve resistance to deactivation opening the opportunity to lower noble metals content. Successful practical achievements were obtained but explanations given for their origin led to strong debates.

This talk will show that the method for palladium incorporation, e.g. one-pot synthesis versus sequential method, is a critical step in optimizing catalytic performances as the stability of metal-support interaction, that can prevent Pd particles sintering in severe operating conditions, can change. The steady-state kinetic measurements will be discussed on fresh and aged catalysts in the light of the physico-chemical characterization showing, according to the preparation method, a disturbance in the kinetics of the reaction linked to different mechanisms and associated with a surface restructuring provoked by exsolution and coalescence processes.

Biography:

Pascal GRANGER studied at the university of Poitiers (France) and obtained is PhD degree in applied chemistry in 1992. He became Lecturer in 1994 and became full professor in 2003 at the university of Lille. His fields of expertise are focused on the kinetics of catalytic reactions and related mechanisms, the coupling between spectral and kinetic features, the understanding of ageing processes of heterogeneous catalysts in working conditions. His current interest also concerns the development of perovskite type oxides in postcombustion catalysis. His co-authored of more than 150 full papers, 8 chapters books and guest editor of 4 books.

Hydrogen Spillover. The Forgotten Chemistry

Mohammed Bettahar

Lorraine University, France

Abstract Not Available!!!

A novel titanium dioxide immobilized on stainless steel slag: synthesis, electrochemical characterization and NOx abatement

Siaw Foon Lee*
Lorenzo Plaza
Eva Jimenez-Relinque
Marta Castellote

The Eduardo Torroja Institute for Construction Science (IETcc), CSIC, Madrid, Spain

Abstract:

Efforts have been made to search for denitrification technologies to reduce nitrogen oxides (NO_x) generated by automobile engines and fossil fuel combustion for the protection of human health [1-3]. As far as our knowledge, the use of titanium dioxide (TiO_2) coated on stainless steel slag (SSS) without acid-base treatment for NO_x removal has not been reported yet. In this study, a synthesis of P25 TiO_2 (of 15%, 25%, 35%, 50%, 75% and 100%) and SSS composite was developed. SEM-EDX mapping and XRD revealed that the developed synthesis allowed P25 to be successfully coated on SSS. The data of NOx removal showed that the replacement of P25 by SSS can be done up to 65% without losing the photocatalytic ability in NO_x abatement. Electrochemical characterization revealed that no surface states were detected and electron lifetime was the same for all P25/SSS composites, not affected by the percentages of SSS incorporated. Band structures (conduction band and valence band) of all P25/SSS composites constructed from flat band potentials obtained from Mott-Schottky analysis presented excellent photocatalytic abilities in all P25/SSS composites in NOx abatement, which is in agreement with the observation from the data of NOx removal. This research sheds light on the newly developed synthesis that allows P25 to be immobilized on the untreated SSS and the reuse of the raw SSS in an economic way for the environmental issue.

Chemical and structural properties of graphene – influence of reducing conditions

Beata Lesiak-Orłowska

Institute of Physical Chemistry Polish Academy of Sciences, Warsaw, Poland

Abstract:

Reduced graphene oxide (rGO) was prepared by chemical reduction of graphene oxide (GO) (with a modified Hummers method) in aqueous solutions of different strong and weak reducing agents, and also accompanied by a microwave treatment at 250◦C (MWT) and by a high pressure microwave reactor (HPMWR) at 55 bar [1,2]. GO and received rGOs were investigated by XPS/XAES supported by TEM, XRD, Raman, IR, and REELS. The GO and rGOs' stackingnanostructure (flake) size, interlayer distance, average number of layers in flakes, distanc between defects, elementary composition, content of oxygen groups, C sp3 and vacancy defectswere determined. The average number of flake layers obtained from XRD and REELS wasconsistent. The thinnest flakes rGO obtained using sodium borohydride exhibits the largest content of vacancy, C sp3 defects and hydroxyl group accompanied by the smallest content of epoxy, carboxyl and carbonyl groups due to a mechanism of carbonyl and carboxyl group reduction to hydroxyl groups. The number of layers in rGOs increases with decreasing content of vacancy, C sp3 defects, oxygen groups, water and flake diameter. MWT conditions facilitate formation of vacancies and additional hydroxyl, carbonyl and carboxyl groups at these vacancies, provide no remarkable modification of flake diameter, what results in more competitive penetration of reducing agent between the interstitial sites than via vacancies.

Biography:

Beata Lesiak-Orłowska Completed PhD in physical and theoretical chemistry (Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw, Poland). Post-doctorate at Department of Chemistry, University of Cambridge, UK. Habilitation in physical sciences (Department of Physics and Astrophysics, University of Wrocław, Poland). Coauthor of 130 publications at international journals (few under preparation), 1 patent, 154 international conference contributions and 19 invited. Number of citations 3216, H-index 23 (Scopus). The member of International Advisory Committee at ECOSS. Editorial Board Member of Recent Patents on Materials Science.

Guest Editor in Catalysts MDPI Special Issue "Surface Chemistry in Catalysis" (2020), "Surfaces and Interfaces in Biocatalysis" (2022).

Rare-Earth MOF Derived Catalysts For The RWGS Reaction

Raluca L. Vasile[1]*
Carlos Martínez Gómez[2]
Belén Bachiller Baeza[2]
Felipe Gándara[1]
Consuelo Álvarez Galván[2]

[1]Materials Science Institute of Madrid (ICMM-CSIC), Spain
[2]Catalysis and Petrochemistry Institute (ICP-CSIC), Spain

Abstract:

The rising global energy demand and the unceasing emission of greenhouse gasses into the atmosphere are alarming environmental issues. In order to mitigate the effects of climate change, the emissions of one of the main greenhouse gasses, CO_2, must be reduced. The reverse water-gas shift (RWGS) reaction is one of the most important industrial reactions that utilizes CO_2 as a reactant, catalytically reducing it into carbon monoxide and water. In the quest for sustainable, cost-effective and high efficiency catalysts for this reaction, metal-organic frameworks (MOFs) arise as a new trend. MOFs are a class of reticular multifunctional materials, that consist in metal centers bonded to organic linkers, generating extended networks with desired topological and geometrical features. However, the high temperature requirements for RWGS reaction precludes from direct use of MOF catalysts. Nevertheless, they provide a unique platform to create other type of solids through their thermal transformation. The main advantage of using MOF-derived materials is that it is possible to access structural and compositional features that cannot be obtained through conventional synthetic routes. Previous studies showed that CeO_2 has great effectivity in activating CO_2 molecules, therefore it is a good catalyst for RWGS. Additionally, Ni has been found to rise the conversion rate of CO_2. Bearing this in mind, we used a rare-earth MOF family as a precursor for obtaining rare-earth-doped CeO_2 and Ni-doped La_2O_3. These newly synthesized materials have exhibited excellent catalytic activity in RWGS, with quantitative selectivity to CO and conversion rates rivaling those of commercial catalysts.

Biography:

Raluca L. Vasile is currently a 4th year PhD student in the Multifunctional and Supramolecular Materials group at the Materials Science Institute of Madrid (ICMM-CSIC) in Spain. Her work is focused on the synthesis and chemical and structural characterization of single metal and multimetal MOFs. Additionally, she is also studying the performance of these materials in several applications such as catalysis and magnetism.

Heterogeneous Catalysis with Non Critical Materials for Energy and Environmental Applications

Lucia D'Accolti

University of Bari, Italy

Abstract Not Available!!!

Effects of Zr addition on the refinement of θ-$Al_{13}Fe_4$ and α-Al in an Al-4Fe alloy

Junhai Xia, Zhongping Que*
Chamini L. Mendis
Zhongyun Fan

Brunel Centre for Advanced Solidification Technology (BCAST), Brunel University London, Uxbridge, Middlesex UB8 3PH, UK

Abstract:

The refinement of Fe-containing intermetallic compounds (FIMCs) is important as coarse FIMCs has detrimental effects on the mechanical properties of Al alloys. In this study, the effects of Zr addition on the refinement of θ-$Al_{13}Fe_4$ were investigated with SEM and XRD and validated. The results showed that with a 0.5 wt.% Zr addition to Al-4Fe alloy, both the primary θ-$Al_{13}Fe_4$ and the α-Al grains were significantly refined. Different types of Al-Zr compounds which form as the primary phases before the solidification of θ-$Al_{13}Fe_4$ were observed. The Al_3Zr particles with a cuboidal morphology are the major Al-Zr compound which contributed to the refinement of both the α-Al grains and the primary θ-$Al_{13}Fe_4$ in Al-4Fe alloy. The grain refinement mechanisms and the relationship among the Al_3Zr, θ-$Al_{13}Fe_4$ and α-Al were investigated.

Biography:

She is a research fellow of BCAST at Brunel University London. She is playing a leading role in the area of understanding heterogeneous nucleation mechanism and developing grain refiner for the Fe-containing intermetallic compounds in the recycled Al alloys. Her research interests lie in some other relative area such as multi-crystal transformation, in-situ solidification process. She developed a new approach to grain refine intermetallic compounds by interfacial segregating constitute elements of compounds. She developed a new concept of "composition templating" for heterogeneous nucleation of intermetallic compounds.

Decentral Hydrogen

Paul Grunow[1]*

Trinity Solarbeteiligungen, Germany

Abstract:

Decentral hydrogen is introduced as fast transition path to short and long-term power storage. It circumvents slow infrastructure installments and enables on-site storage and heat coupling in addition to direct use of local electric power. The power-to-gas approach is extended to small combined heat and power devices in buildings that alternately operate fuel cells and electrolysis. While their heat is used to replace existing fossil heaters on-site, the power is either fed into

the grid or consumed via heat-coupled electrolysis to balance the grid power at the nearest grid node. In detail, the power demand of Germany is simulated as a snapshot for 2030 with 100% renewable sourcing. The standard load profile is supplemented with additional loads from 100% electric heat pumps, 100% electric cars, and a fully electrified industry. The renewable power is then scaled up to match this demand with historic hourly yield data from 2018/2019. An optimal mix of photovoltaics, wind, biomass and hydropower is calculated in respect to estimated costs in 2030. In most master plans, hydrogen is understood to be a substitute for fossil fuels. This talk focuses on hydrogen as a storage technology in an all-electric system. The target is to model the most cost-effective end-to-end use of local renewable energies, including excess hydrogen for the industry. The on-site heat coupling is the principal argument for decentralization here. Essentially, it flattens the future peak from exclusive usage of electric heat pumps during cold periods. Batteries are tried out as supplementary components for short-term storage, due to their higher round trip efficiencies. Switching the gas net to hydrogen is considered as an alternative to overcome the slow infrastructure expansions. Further decentral measures are examined in respect to system costs.

Biography:

Paul Grunow has completed his Ph.D at the age of 30 years from Technical University Berlin and Helmholtz-Zentrum Berlin and postdoctoral studies from the COPPE/UFRJ in Rio de Janeiro, Brazil. He is the general manager of Trinity Solarbeteiligungen GmbH, an investment company in renewable energies. Before, he co-founded three companies in the area of photovoltaics based in Berlin, i.e. Solon, Q-Cells, PI Photovoltaik-Institut Berlin. He has published more than 12 papers in reputed journals.

Polyhydroxybutyrate/polyethylene glycol/TiO2:Sm3+ composites for methylene blue dye degradation

Maraolina Domínguez-Díaz*
José Escorcia-García
Arizbe Chavéz-Pérez

Cinvestav Unidad SaltilloRamos Arizpe, Coahuila 25900, México.

Abstract:

In this work, polyhydroxybutyrate (PHB)/polyethylene glycol (PEG)/TiO2 and PHB/PEG/TiO2:Sm3+ composites in films and membranes are prepared by using cast film and centrifugal spinning techniques. The TiO2:Sm3+ particles are obtained through the sol-gel route. The polymers, photocatalytic particles, and composites are analyzed with the help of XRD, SEM, sessile drop technique, luminescence, and UV-visible spectroscopy. The PHB and PEG polymers have an orthorhombic and monoclinic crystalline phase, respectively, while TiO2 particles are constituted by the anatase and rutile crystalline phases. The doping of TiO2 with Sm3+ stabilizes the anatase crystalline phase, reducing the rutile phase content. The UV-visible spectra results show that doping increases titania's optical bandgap (Eg) from 3.07 to 3.18 eV for TiO2 and TiO2:Sm3+ , respectively. The increment is occasioned by the reduction of the crystallite size (D) and crystallinity. SEM's elemental mappings of film and membrane composites present a homogeneous distribution of TiO2 and TiO2:Sm3+ photocatalytic particles embedded in the polymer matrix. Moreover, the wettability of composites decreases with the addition of photocatalytic particles. In addition, the surface free energy of the membrane composites is lower (by approximately 30 mJ/m2) than those obtained in film. The composite with the highest methylene blue dye degradation under UV light was the membrane constituted with TiO2/Sm3+ , which degrades the dye (c/c0≈0) in about 90 minutes. On the contrary, the composites with the lowest dye degradation

are the polymer film (c/c0≈0.53) and the polymer membrane (c/c0≈0.62). These results indicate that the PHB/PEG/TiO2:Sm3+ composites are suitable for degrade dyes in an aqueous solution.

Biography:

Maraolina Domínguez-Díaz has a bachelor's degree in Physics from the Juárez Autonomous University of Tabasco, Mexico. She completed a Master's in Engineering and Applied Sciences with a specialization in Materials Technology from the Autonomous University of the State of Morelos (UAEM), Mexico. Later, she obtained her Ph.D. degree in Engineering and Applied Sciences with a specialization in Electrical Technology from the UAEM. Afterward, Dr. Domínguez-Díaz did post-doctoral research at the Institute of Physical Sciences of the National Autonomous University of Mexico. Later, she did another post-doctoral research in the Cinvestav, Mexico. Her research is about polymer/ceramic composites for different applications.

Multifunctional Separators for Improved Li-Ion Batteries Durability

Ion C. Halalay[1]*
Anjan Banerjee[2]
Baruch Ziv[2]
Yuliya Shilina[2]
Shalom Luski[2]
Doron Aurbach[2]
Hanshuo Liu[3]
Kristopher J. Harris[3]
Gianluigi Botton[3]
Gillian R. Goward[3]

[1]General Motors R&D, Warren MI, USA
[2]Bar-Ilan University, Ramat-Gan, Israel
[3]McMaster University, Hamilton, Ontario, Canada

Abstract:

Dissolution of manganese and other transition metal ions from positive electrodes, and the loss of electroactive Li^+ ions are two main causes for reduced Li-ion batteries (LIBs) durability. Parasitic reactions involving acid species also cause performance degradation in LIBs that are not affected by Mn dissolution. I will discuss progress in the understanding of Mn species in LIBs and two mitigation measures for LIB degradation: trapping of dissolved transition metal (TM) ions and scavenging of acid species by multifunctional separators (MFSs). MFSs increase the capacity retention during prolonged electrochemical cycling of LIBs and improve their rate performance. The electrochemical performance of cells was evaluated by constant current cycling and electrochemical ac impedance spectroscopy (EIS). Harvested cell components were analyzed by XRD, ICP-OES, XANES, HR-SEM, FIB-SEM, and MAS-NMR. EIS data show that, after cycling, the interfacial and ion-transfer resistances of anodes and positive electrodes from $LiMn_2O_4$-graphite cells are considerably smaller in cells with MFSs than in cells with plain separators. FIB-SEM data show a smaller average film thickness on graphite electrodes from cells with MFSs than with baseline separators. Saturation of the MFSs with Mn ions does not increase the capacity fade rate during cell cycling. EDX and ^{19}F MAS-NMR data indicate qualitative differences in the chemical make-up of electrode films: different F:P ratios and LiF amounts in graphite electrodes harvested from $LiMn_2O_4$-graphite cells with MFSs vs. plain separators. Acid-scavenging MFSs improve the cycle life of $LiNi_{0.5}Mn_{1.5}O_4$-graphite cells and they also benefit cell chemistries not affected by TM dissolution, like $LiNi_{0.6}Mn_{0.2}Co_{0.2}O_2$-graphite.

Biography:

Ion C. Halalay received a M.Sc. degree in Physics from the University of Bucharest, Romania, in 1980, and a Ph.D. in Physics from the Massachusetts Institute of Technology in 1991. He joined General Motors R&D in 1982, where he has performed research on Li-ion batteries, PEM fuel cell materials, in-situ engine oil diagnostics, the sonochemical production of metal powders, plasma-jet ignition of transient flames, and the production of metallic glasses. His work has resulted in 48 US patents and 58 peer reviewed publications. Over the past decade, his research focused on functionalized separators and battery anodes containing Si-based materials.

Lithium superoxide stabilization through Ir3Li and implication toward high energy capacity Li-O2 batteries

Hsien-Hau Wang

Materials Science Division, Argonne National Laboratory, USA

Abstract:

Developing batteries with comparable energy densities to internal combustion technology is essential to fully transition to an electrified transportation-based society. Li-O2 batteries, are seen as the 'holy grail' of battery technologies since they have the highest theoretical energy density of all battery technologies. Current lithium-oxygen (Li-O2) batteries suffer from large charge overpotentials related to electronic resistivity of the insulating lithium peroxide (Li2O2) discharge product. One potential solution is the formation and stabilization of lithium superoxide (LiO2) discharge intermediate that exhibits metallic conductivity. Cathodes based on small iridium nanoparticles have been used in a Li-O2 battery to form LiO2, however, it has a short lifetime. We found that the LiO2 was stabilized on Ir3Li surfaces which were generated from Ir nanoparticles during battery cycling. We studied the electronic properties of Ir3Li, which was thermally synthesized in bulk. The bulk Ir3Li powders were found to have comparable electrical conductivity to Ir metal, possessed metal-like magnetic properties, and had an affinity towards O2 adsorption. The LiO2 formed from the Li-O2 battery discharge was characterized using Raman, titration, and transmission electron microscopy. This analysis revealed the formation of ultra-nanocrystalline LiO2 particles > 200 nm. This result was attributed to the use of large micron sized Ir3Li particles, which could stabilize larger LiO2. These results demonstrate that cathode properties can be modified to stabilize the bulk LiO2 discharge product, which will be useful for further development of LiO2-based Li-O2 batteries. This work was supported by the US DOE under Contract No. DE-AC02-06CH11357 from the Vehicle Technologies Office, Office of EERE.

Biography:

Hsien-Hau Wang obtained his BS (Chemistry, '75) from the National Tsing-Hua University, Taiwan, and his PhD (Inorganic/Organometallic Chemistry, '81) from the University of Minnesota, Minneapolis, MN. He was a postdoctoral fellow at the University of Illinois, Urbana, IL with Prof. K. Suslick (Sonochemistry, '83). Since then, he joined the Argonne National Laboratory, Materials Science Division. He has been working on Organic Conductors and Superconductors, Anodized Aluminum Oxide based nanoscience and membrane catalysis. His current research is in Li ion and Li-oxygen batteries for energy storage.

Distal Functionalization via Transition Metal Catalysis

Haibo Ge

Department of Chemistry & Biochemistry, Texas Tech University, Lubbock, TX, USA

Abstract:

The ubiquitous presence of sp^3 C–H bonds in natural feedstock makes them inexpensive, easily accessible, and attractive synthons for the preparation of common and/or complex molecular frameworks in biologically active natural products, pharmaceutics, agrochemicals, and materials. However, the inertness of these bonds due to the high bond dissociation energies and low polarity difference between the carbon and hydrogen atoms makes them challenging reaction partners. Moreover, the desired site-selectivity is often an issue in reactions with multiple analogous sp^3 C–H bonds. To overcome these problems, transition metal-catalyzed C–H functionalization has been developed with the assistance of various well-designed directing groups which can coordinate to a metal center to deliver it on a targeted C–H bond through an appropriate spatial arrangement, enabling C–H activation via the formation of a cyclometalated species. However, the requirement of often additional steps for the construction of the directing groups and their subsequent removal after the desired operation severely hampers the efficacy and compatibility of the reactions. A promising solution would be the utilization of a transient ligand which can bind to the substrate and coordinate to the metal center in a reversible fashion. In this way, the directing group is installed, sp^3 C–H functionalization occurs, and the directing group is then removed *in situ* without affecting the substrate function after the catalysis is finished. Overall, the whole process occurs in a single reaction pot. Herein, we are presenting our studies on transition metal-catalyzed transient directing group-enabled C–H functionalization reaction.

Biography:

Haibo Ge received his PhD degree in Medicinal Chemistry from The University of Kansas in 2006, and then moved to The Scripps Research Institute for postdoctoral study. In 2009, he began his independent academic career at the Indiana University – Purdue University Indianapolis and relocated to Texas Tech University in 2020. Research by his group is mainly focused on the development of novel methods for carbon–carbon and carbon–heteroatom bond formation through transition metal catalyzed C–H functionalization.

Catalytic reactivity of Pd-Cu/Al_2O_3 for catalytic hydrogen combustion

Jongho Kim[1]*
Arash Tahmasebi[1]
Soonho Lee[1]
Chung-Hwan Jeon[2]
Jianglong Yu[3]

[1]University of Newcastle, Australia
[2]Pusan National University, South Korea
[3]Monash University-Southeast University Joint Graduate School, China

Abstract:

Catalytic hydrogen combustion (CHC) is a promising technology for clean, efficient, and safe energy generation in hydrogen-fueled systems such as a catalytic combustor (boiler) that gen-

erate water as a product. This research focused on the performance evaluation and catalytic reactivity and stability of Pd-Cu/Al_2O_3 catalyst during CHC at target temperatures (i.e. 500 °C). The physicochemical and catalytic properties of catalysts were characterized by various analytical techniques. The particle size distribution and reducibility of the catalysts were studied to investigate the influence of the catalyst composition on its activity. Higher reduction temperature resulted in a higher fraction of metallic Pd, leading to improved catalytic reactivity at the optimized composition of 0.75Pd0.25Cu/Al_2O_3. The reaction rates were measured using a fixed-bed reactor system connected to a micro-GC and the rate law equations containing the water-related term were determined. The effects of temperature and catalyst composition on reaction mechanism were investigated by in-situ FTIR analysis, which was used to detect the intermediates compounds formed during the catalytic combustion process (i.e. OH). In particular, the generation of OH group and water was analyzed as a means of comparing the reaction pathways over the optimized Pd-Cu bimetallic and monometallic catalysts. In addition, the effects of Cu replacement on catalytic reactivity and stability as well as the reaction pathways of Pd were investigated to understand the catalytic performance of the Pd-Cu catalyst. The determined rate law in this study can be used to design catalytic boilers for domestic heating applications.

Biography:

Jongho Kim is a PhD candidate in the Department of Chemical Engineering at the University of Newcastle. He obtained his Master's degree from the Department of Mechanical Engineering at Pusan National University in 2018. His PhD project is on experimental and numerical evaluation of flameless catalytic combustion of hydrogen. His research focuses on the fundamental investigation of mechanisms, reaction pathways and process optimization of flameless catalytic hydrogen combustion for clean energy generation. He has published a series of peer-reviewed papers on combustion research.

Transition-Metal-Catalyzed C(sp3)–H Carboxylation of CO2

Tsuyoshi Mita

Hokkaido University, Japan

Abstract Not Available!!!

Innovative technologies for eliminating anthropogenic CO2 emission(IPEACE)

Tohru Setoyama*

Mitsubishi Chemical corp. Science & Innovation center, Yokohama, Japan

Abstract:

For realizing carbon neutral for the mitigation of climate change at the middle of this century, chemical industry has a crucial responsibility because it has been providing their products from fossil resources. We have been developing various catalytic technologies as IPEACE since the early of 21st century. They are categorized three types. The 1st one is the switching from processes derived from cracker to those from methane resource. Although reforming of methane, methanol synthesis and MTO seem to be wellestablished, there are many rooms to provide more energy -effective processes. The 2nd is the processes derived from biomass. We argue

olefin production processes from bioethanol and some chemicals, which keep specific chemical structures derived from carbohydrate such as polysaccharide. Even after making best effort to minimize CO2 emission in these categories, we cannot avoid the profile of carbonpositive. For realizing carbon neutral, we need some carbon-negative process as a finishing blow, which can consume CO2 as a chemical resource. As a 3rd category, we have been investigating artificial photo synthesis including catalytic water splitting under visible light and olefin synthesis derived from relevant green hydrogen and CO2. from this aspect. To realize the destructively cheap cost of hydrogen is very key for large-scale application of this technology. We will argue the current status and perspective about them.

Biography:

Tohru Setoyama (Dr. , 64 years old) Joined Mitsubishi chemical at 1983 after getting Master degree of University of Tokyo. His Contribution of commercialization of several technologies: Vapor phase hydrogenation of carboxylic acid by ZrO2 cat. Ring opening polymerization of THF by mesoporous cat. and etc. He is a Project leader of "Artificial photo synthesis" from 2012 to (2030?) and Project officer of JSTCREST "Hyper nano-space design" from 2013 to 2021. Expertise at Design of heterogeneous cat. and of inorganic materials, Chemical Engineering.

Gas-phase Oxidation of Benzene to Phenol over Cu Catalyst Doped on Molding MFI Type Zeolite

Yuichi Ichihashi*
Xindong Yin
Shuhei Miyamoto
Keita Taniya
Satoru Nishiyama

Department of Chemical Science and Engineering, Graduate School of Engineering, Kobe University, 1-1 Rokkodai, Nada, Kobe 657-8501, Japan

Abstract:

The gas-phase benzene oxidation with molecular oxygen to phenol was carried out by using Cu catalyst loading on the molding HZSM-5. This molding HZSM-5 (HBLMFI) was prepared by binder-less HZSM-5 manufacturing method which were reported as the patents from Nippon Shokubai. The catalyst, Cu-HBLMFI, was prepared by doping HBLMFI with Cu by an ion-exchange method.

In order to investigate the influence on the oxidation performance bring out by the size of the catalyst particle, the benzene oxidation was attempted by using the prepared Cu-HBLMFI with a constant contact time and a variable linear velocity. Resultingly, the conversion of benzene was constant at sufficiently high linear velocities. This means that the shape of catalyst and the diffusion in the outer particle boundary film did not affect the activity in this reaction. On the other hand, at slower linear velocities than normally used, the conversion of benzene decreased with decreasing linear velocity. This meaned that at slow linear velocities, the diffusion of the reactants to the grain boundary film became rate determining steps.

Finally, it was clarified that the Cu-HBLMFI catalyst showed almost the same activity as the powder fine particle catalyst. From these results, it was also indicated that the reactants were sufficiently diffused and reacted even within the prepared Cu-HBLMFI catalyst as compared with the powdered Cu/HZSM-5 catalyst.

Biography:

Yuichi Ichihashi is an associate professor of catalysis and catalytic reaction engineering group at Department of chemical science and engineering, Graduate school of engineering, Kobe university. His current research focuses on the direct oxidation from benzene to phenol over the several supported Cu or V catalysts. And he has also investigated about the selective oxidation of several organic compounds and the water cleavage reaction over the metal oxide photocatalysts.

Ionic Liquid Catalyst for Polysaccharide Modification

Daisuke Hirose*

Kanazawa University, Japan

Abstract:

As society is currently dependent on petroleum resources, the development of direct one-step synthesis methods with minimal consumption and disposal for a fully bio-based resin is a critical task. Polysaccharide esters typified by cellulose ester are used as bio-based polymer. They consist of cellulose, which is the most abundant natural polymer; however, the condensation reactions between cellulose and carboxylic acids consume condensation reagents and generate corresponding waste. In this study, a method of polysaccharide modification involving simply mixing polysaccharide typified by cellulose with natural aldehydes contained in essential oils, as represented by α,βunsaturated aldehyde "cinnamaldehyde" known as cinnamon flavor, in an ionic liquid has been developed.1,2 An oxidative esterification reaction proceeds between polysaccharide and cinnamaldehyde to directly provide the highly substituted and formally fully bio-based polysaccharide ester with perfect atom economy and without additional reagents and catalysts.

Biography:

He is Assistant Professor in the Prof. Katsuhiro Maeda group at Kanazawa University. He received his B.S. (2011), M.S. (2013) and Ph.D. (2016) degrees from Kanazawa University in the group of Prof. Hiroyuki Ishibashi and Shigeyoshi Kanoh. After spending three years in Prof. Katsuhiro Maeda and Prof. Kenji Takahashi groups as a postdoctoral researcher and Research Assistant Professor, he joined the Maeda group in the current position in 2019. His current research interests are green chemistry and polymer chemistry.

Development of ionic liquid-based mixed matrix membrane for CO_2 separation

Nor Naimah Rosyadah Ahmad[1]*
Choe Peng Leo[2]
Abdul Wahab Mohammad[1]

[1]Department of Chemical and Process Engineering, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, Bangi, Selangor, Malaysia

[2]School of Chemical Engineering, Engineering Campus, Universiti Sains Malaysia, Nibong Tebal, Penang, Malaysia

Abstract:

Carbon capture and storage (CCS) technologies have gained global attention due to the environmental impact caused by CO_2. Ionic liquid, also known as a designer solvent, has good potential for CO_2 capture application due to its good CO_2 affinity, negligible vapor pressure and high thermal stability. The combination of ionic liquid and membrane technology has been introduced for the more effective use of ionic liquid. This work provides an overview of mixed matrix membrane (MMM) and the application of ionic liquid in the membrane for CO_2 separation, focusing on recent advances in ionic liquid- based MMM. Descriptions of various MMM modification strategies using ionic liquid and the influence of challenging operating conditions on the CO_2 separation performance of ionic liquid-based MMM are discussed.

Biography:

Nor Naimah Rosyadah Ahmad holds a PhD in Chemical Engineering from Universiti Sains Malaysia. Her PhD research focused on developing ionic liquid-based composite membrane for CO_2 capture application. Currently, Naimah is a postdoctoral researcher in the Department of Chemical and Process Engineering, Universiti Kebangsaan Malaysia. Her main fields of scientific interest include membrane technology, advanced materials for CO_2 capture (e.g. ionic liquid, deep eutectic solvent, zeolite, graphene, metal-organic framework), gas separation, wastewater treatment, and climate change mitigation. She has participated in various international invention expositions and received several prestigious awards at the national and international levels, including the Travel Awards from the European Membrane Society (EMS) and the Institute of Advanced Sustainability Studies (Postdam, Germany).

Manufacturing of Large Area Solid-state Nanopore Array

Jufan Zhang[1]*
Hongshuai Liu[1]

Centre of Micro/Nano Manufacturing Technology, School of Mechanical and Materials Engineering, University College Dublin, Ireland

Abstract:

Nanopore brings extraordinary properties for a variety of potential applications in various industrial sectors. Since manufacturing of solid-state nanopore was firstly reported in 2001, solid-state nanopore has become a hot topic in the recent years. An increasing number of manufacturing methods have been reported, with continuously decreased sizes from hundreds of nanometres at the beginning to approximate one nanometre until recently. To enable more robust, sensitive, and reliable devices required by the industry, researchers have started to explore the possible methods to manufacture nanopore array which presents unprecedented challenges on the fabrication efficiency, accuracy and repeatability, applicable materials, and cost. As a result, the exploration of fabrication of nanopore array is still in the fledging period with various bottlenecks. This presentation introduces an efficient and cost-effective manufacturing process chain for fabricating large area solid state nanopore array. The authors successfully fabricated the 20 nm nanopore array in a 15 mm × 15 mm area, with relatively uniform pore shape and size. The experiments also indicated a possible way to reduce the pore size down to 1nm simultaneously modify the geometry of nanopore channel, which would be a breakthrough to facilitate the high-resolution DNA sequencing. Some representative applications of nanopore array include DNA/RNA sequencing, energy conversion and storage, water desalination, nano-sensors, nanoreactors and dialysis.

Biography:

Jufan Zhang, Assistant Professor in School of Mechanical and Materials Engineering, Principal Investigator in Centre of Micro/Nano Manufacturing Technology, University College Dublin, Ireland. He leads the research in manufacturing of solid state nanopore array and corresponding biomedical applications. He has chaired 10+ research funding, and made 50+ peer-reviewed publications and 7 patents. He is the Member of Irish Manufacturing Council, International Academy of Engineering and Technology, International Society for Nanomanufacturing. He is the Chair of Organizing Committee of the 8th International Conference on Nanomanufacturing and the 4th AET Symposium on ACSM and Digital Manufacturing.

PMMA Composite Films for Electrochromic Glass Using Ultrasonic Spray Technique

Chi-Ping Li[1]*
Bing Ze Li[1]

[1]Department of Chemical Engineering, National United University, Miaoli, Taiwan

Abstract:

In this research, ultrasonic spray deposition (USD) technology was used, with polymethyl methacrylate (PMMA) as the matrix, dimethyl carbonate (DMC) as the solvent, and silicon dioxide as the second phase to prepare nanocomposite polymer electrolyte membranes. The nanocomposite polymer solution was deposited using a model 8700-120 spray head (Sono-Tek Corporation) at a frequency of 120 kHz. The annealing procedure improves the uniformity and transmittance of the film. Due to the aggregation of silica nanoparticles, the addition of silica reduces the transmission of the electrolyte membrane. However, the addition of the surfactant cetyltrimethylammonium bromide (CTAB) disperses the silica nanoparticles and returns the optical transmittance of the nanocomposite polymer electrolyte membrane to about 90%. The transmission and mechanical properties of nanocomposite polymer electrolyte films based on PMMA and fumed silica nanoparticles deposited by ultrasonic spray deposition were studied. The film transmission is good. The hardness and elastic modulus of our nanocomposite polymer electrolyte membrane are better than commercial materials.

Biography:

Chi-Ping Li received his PhD of Materials Science from Colorado School of Mines (USA) in 2014 and followed by postdoctoral research in National Renewable Energy Laboratory (NREL, USA) in 2015. He joined Department of Chemical Engineering in National United University in Taiwan as an assistant professor in 2018. His research interests are mainly focused on synthesis of nanostructured films, nanocomposite films and nanoparticles. Those materials are used in electrochromic windows, lithium batteries, organic photovoltaics and LED encapsulants. His goal is to overcome the challenges and produce great but low cost materials in the fields of green and renewable energy.

Biodiesel Production in Continous and Semicontinous Ultrasonic Reactor

Francisco Rodriguez

CIDETEQ, Mexico

Abstract Not Available!!!

Study on wave function and reactivity of carbon on the active metal doped armchair edges and chemisorption of carbon

Jie Zhang[1]*
Shiqiang Zhan[1]
Xudong Song[2]
Baohuan Wei[3]
Bo Wang[1,4]

[1]School of Energy and Power Engineering, University of Shanghai for Science and Technology, Shanghai 200093, China
[2]State Key Laboratory of High-Efficiency Utilization of Coal and Green Chemical Engineering, Ningxia University, Yinchuan 750021, China
[3]Shanghai Institute of CleanTech Innovation, Shanghai, 201600, China
[4]Shanghai Key Laboratory of Multiphase Flow and Heat Transfer in Power Engineering, Shanghai, 200093, China.

Abstract:

The molecular reactivity and CO_2 chemisorption properties of the armchair-edge carbon models doped with calcium/potassium were studied by using wave function theory and density functional theory. Comparing the electronegativity, electrophilicity, and nucleophilicity of several models leads to the conclusion that the chemical adsorption of carbon dioxide on the armchair carbon edge is an electrophilic reaction process. Electrons are transferred to carbon dioxide during chemisorption. Frontier molecular orbital theory, electron localization function, and electron density difference of the carbonization model with armchair edge were analyzed. Compared with the single metal doped edge, the bimetal doped edge was filled with more lone pairs of electrons, making the carbon edge more favorable to electrophilic attacks. Through a comprehensive analysis of the double descriptors and Hirshfeld atomic charges of different models, the specific adsorption sites of CO_2 were predicted, which were more likely to be chemically adsorbed at the edge rather than above the carbon plane. At the B3LYP and revDSD-PEBP86 level of theory, combined with D4 dispersion correction, the energies released by the chemisorption of CO_2 in different modes were calculated respectively. An active form of the non-linear structure of CO_2 was confirmed. The thermodynamic results were consistent with the predictions of wave function theory and density functional theory.

Biography:

Jie Zhang is working in the School of Energy and Power Engineering at the University of Shanghai for Science and Technology. His research focuses on the interface of heterogeneous catalysis, utilization of CO_2 and H_2O, chemical process design, and evaluation of energy efficiency for utilization of biomass/coal. He applies a wide range of synthetic, spectroscopic, and computational chemistry tools to study the chemical transformation of molecules on catalytic surfaces. Research projects are aimed at addressing issues associated with alternative energy, renewable chemicals, and novel catalyst design at the atomic level.

Design and Synthesis of Merrifield Resin-Supported Binuclear Dioxidovanadium(V)

Complexes for the Solvent-Free Catalytic Oxidation of Light Aliphatic Alcohols

Chanchal Haldar

Indian Institute of Technology (Indian School of Mines) Dhanbad, India

Abstract Not Available!!!

Efficiency of Iron Nickel Bimetallic Catalysts in Chemoselective Hydrogenation of Carbonyl Compounds

Muhammad Sadiq[1,3,*]
Umar Wahab[1]
Zaffar Iqbal[2]
Saima Sadiq[3]
Chang Min Kim[3]
Sher Ali Khan[3]

[1]Department of Chemistry, University of Malakand, Chakdara-18800, Pakistan
[2]Department of Chemistry, Bacha Khan University, Charsadda-24420, Pakistan
[3]Department of Chemistry, Kyungpook National University, Daegu-41566, South Korea

Abstract:

Selective hydrogenation of carbonyl moiety in the presence of olefinic group and other reducible functionality is an industrially important transformation. However, the protocol of green chemistry cannot be forfeited for this formidable challenging transformation. Therefore, iron nickel bimetallic recyclable catalyst (Fe/Ni) was used for base free hydrogenation of carbonyl compound with high activity and chemoselectivity in microwave environment. Microwave irradiation, amount of dopant and pre-treatment of catalyst (Fe/Ni) divert conversion/selectivity toward C=O group as compared to C=C or another reducible moiety. The pyridine adsorption studies revealed that pre-treated catalyst with optimal dopant (Fe) possess more acidic sites as compared to untreated catalyst. Furthermore, the selectivity of bimetallic catalysts towards hydrogenation of carbonyl function group was correlated with Fe content present in the matrix of catalyst using combinatorial approach of theory and experiments.

Biography:

Muhammad Sadiq received his PhD degree with specialization in Physical Chemistry in 2009. He joined Department of Chemistry, University of Malakand as Assistant Professor. Now, he is working as a professor in the same Department. During his career, he worked on diverse funded projects to address challenges across physical chemistry, green and sustainable chemistry, material science and reactor engineering, including hydrogenation/ dehydrogenation of ketone/alcohol in liquid/gas phase, photocatalytic oxidation of alcohols, hydrogen production, utilization of carbon dioxide, and application of novel materials.

Iron based Core-Shell Catalysts for Fischer-Tropsch Synthesis in 3D Printed SS Microchannel Microreactors

Meric Arslan[1]*
Sujoy Bepari[2]
Debasish Kuila[1, 2]

1 Department of Applied Science and Technology, North Carolina A&T State University, Greensboro, North Carolina, 27411, United States
2 Department of Chemistry, North Carolina A&T State University, Greensboro, North Carolina, 27411, United States

Abstract:

Fischer Tropsch Synthesis (FTS) using syngas, a mixture of carbon monoxide (CO) and hydrogen (H_2), in the presence of a catalyst, is an excellent route to long-chain hydrocarbons and fuels. Our research group is focused on synthesizing core-shell nanocatalysts for FTS using CO_2 enriched syngas in 3D printed SS microchannel microreactors. Three different core-shell catalysts Fe_2O_3@SiO_2, Fe_3O_4@SiO_2 and FeCo@$SiO_2Al_2O_3$ were prepared and characterized by N_2 physio-sorption, XRD, SEM, TEM and H_2-TPR techniques. While Fe_2O_3@SiO_2 was prepared by autoclave technique, FeCo@$SiO_2Al_2O_3$ and Fe_3O_4@SiO_2 were prepared by one pot procedure. The surface area of Fe_2O_3@SiO_2, 617m^2/g, is greater than that of FeCo@$SiO_2Al_2O_3$, 241 m^2/g and Fe_3O_4@SiO_2, 106 m^2/g. The surface area decreases upon addition of Al_2O_3 in the shell part of FeCo@$SiO_2Al_2O_3$ catalyst. The XRD studies of Fe_3O_4@SiO_2 and Fe_2O_3@SiO_2 exhibits the respective peaks for the metal. The core-shell structure was observed with some agglomerations in the SEM of Fe_3O_4 based catalyst. The mesoporous hexagonal structure ensures the improvement of diffusion of reactants and products as well as enhanced heat transfer, which is significant for exothermic FTS reactions. The novel material's feasibility as the catalyst for FTS in 3D printed stainless steel microchannel reactors was studied in the temperature range of 200-350°C at 20 bar with H_2/CO molar ratio of 2:1. Fe_2O_3@SiO_2 yields higher conversion than Fe_3O_4@SiO_2, and Fe_2O_3@SiO_2 has higher C_{4+} and C_2-C_4 selectivity than that observed with FeCo@$SiO_2Al_2O_3$.

Biography:

Meric Arslan is a PhD candidate in Applied Science and Technology department of North Carolina A&T State University. He received a bachelor's degree in Mining Engineering from Dumlupinar University in Kutahya, Turkey and a master's degree in Materials Science and Engineering from Norfolk State University in Norfolk, Virginia, USA. He is working in Dr. Kuila's research group and his primary research interests are Core-Shell catalysts for Fischer-Tropsch synthesis. He is focusing on the development of efficient and stable catalysts for Fischer-Tropsch synthesis using CO_2 enriched syngas in 3D printed stainless steel microchannel microreactors.

Plasma-catalytic processes for sustainable future

Kostya (Ken) Ostrikov

Queensland University of Technology, Brisbane, Australia.

Abstract:

This presentation focuses on the role of plasma science and nanotechnology in the field of sustainable and green technological solutions for our planet. Here we introduce several plasma-electrified, plasma-catalytic, and hybrid (synergistic) processes aimed for applications in clean energy, green chemistry and other relevant fields. The urgent need for this research is highlighted by the 26th Climate Change Conference of the United Nations (Glasgow, UK, 31 Oct – 12 Nov 2021) and the key Sustainability Goals of the UN. The presented cases focus on the enabling role of the plasma-aided nanotechnology. The details of the fabrication of high-performance catalysts, electrodes, advanced energy materials and devices, innovative membranes, desalination of sea water and the associated resource recovery, production and storage of clean energy, capture and conversion of greenhouse gases (GHG) to value-added fuels and chemicals, and some other examples. The crucial role of the plasma and nano- technologies is explained for contributing to the future low-carbon-emissions technologies, which are of most interest to the industry sectors which generate most of the GHG emissions. Examples include production of agricultural fertilizers, cement and concrete, steel, iron and other metals, plastics, and also medical and health related products. Decarbonizing the key industry sectors necessitates electrification of the production of materials, chemicals, and fuels. The *re-carbon – de-carbon – up-carbon* sustainable cycle can be achieved using the plasma-enhanced Power-to-X(Products) approach, using clean renewable power. The applications of plasma-power for evolving and expanding such sustainable processes and technologies are discussed as well.

Biography:

Academician Professor Kostya (Ken) Ostrikov is a prolific cross-disciplinary researcher, collaborative research catalyst, enthusiastic community leader, specializing in the plasma and nanotechnology fields. His achievements over 24 active career years include an H-index of 84, with over 32,000 (>18,000 since 2017) citations (Google Scholar); multiple high-profile honours, fellowships and awards, e.g., the recent Humboldt Prize/Award (2021-26), election as a Foreign Fellow of the European Academy of Sciences and Academia Europaea. He is renowned for the studies of plasma effects in the formation and modification of matter with nanoscale features. He engaged, led, mentored and supervised or co-supervised >70 postdoctoral and higher-level researchers, and >100 students.

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UNITED SCIENTIFIC GROUP (A non profit organization)
8105, Suite 112, Rasor Blvd, Plano, TX 75024, USA

Ph: +1-469-854-2280/81
Toll Free: +1-844-395-4102

Email: catalysis@uniscigroup.org
Web: https://catalysis.unitedscientificgroup.org/