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ABSTRACT BOOK

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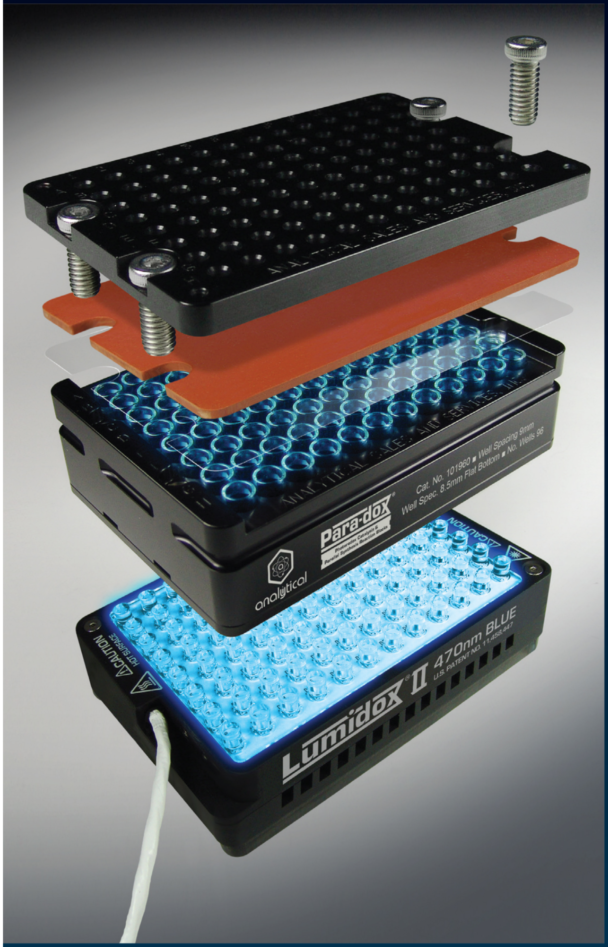

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Metal Complexes Supported on Chloromethylated Polystyrene Cross-linked with Divinyl Benzene as Catalysts for Multicomponent Reaction

Mannar Ram Maurya

Indian Institute of Technology Roorkee, India

Abstract Not Available!!!

Recent Advances in the Preparation and Application of Photocatalysts.

Jimmy C. Yu

The Chinese University of Hong Kong, Hong Kong

Abstract Not Available!!!

Rational Mechanism-Based Catalyst Design for Waste Polymer Recycling in a Circular Economy

Tobin J. Marks

Northwestern University, Evanston, IL

Abstract Not Available!!!

Mechanisms and Rates for Catalytic Reactions Based on Quantum Mechanics and Reactive Force Fields

William A. Goddard III

California Institute of Technology, Pasadena, CA

Abstract Not Available!!!

Oral Presentation

Porous Metal Oxide Catalysts

Steven L. Suib[1-3]* and Shubhashish Shubahshish[1]

Department of Chemistry,[1] Department of Chemical and Biological Engineering,[2] Department of Materials Science and Engineering,[3] University of Connecticut, United States.

Abstract:

We will discuss a synthesis method for highly porous molybdenum oxide via molybdenum-oxo cluster formation under acidic conditions providing extraordinary stability. These systems show high valences of molybdenum when compared to commercial materials based on ultraviolet–visible spectroscopy, electron paramagnetic resonance spectroscopy, and X-ray photoelectron

spectroscopy. A 91% bulk orthorhombic molybdenum oxide was observed with powder X-ray diffraction experiments. Hydrogen peroxide in various solvents was used to obtain pore diameters as large as 17.4 nm and pore volumes as large as 0.168 cm^3/g. These systems are excellent catalysts that have high yields of imine via amine coupling. These reactions are first-order and have turnover numbers on the order of 27.93, which slightly decrease to about 22.04 after four cycles of reaction. To initiate the reaction, the catalyst's surface hydroxyl groups in these solid acid catalysts help to jump-start the reaction. Similar porous metal oxides and their catalytic activity will be covered.

Biography:

Steven L. Suib is a Board of Trustees Distinguished Professor and Director of the Institute of Materials Science at the University of Connecticut. Dr. Shubhashish Shubhashish just received his Ph. D. in Chemistry from the University of Connecticut.

Future Opportunities in Chemical Manufacturing

Esther S. Takeuchi,* Kenneth J. Takeuchi, Amy C. Marschilok

Stony Brook University, Stony Brook, NY, USA

Brookhaven National Laboratory, Upton, NY, USA

Abstract:

The energy landscape is undergoing a transformation where the use of fossil fuels is moving toward cleaner forms of energy. Currently, two of the largest energy segments contributing toward emissions are transportation and electricity generation. Emissions from transportation are being minimized through the adoption of electrified vehicles. The efficacy of this solution depends on the availability of portable power in the form of batteries and electricity from clean sources. The adoption of clean electricity generation by wind and solar is a path forward. However, the widespread adoption of clean electricity generation demands energy storage due to the inherent intermittency of wind and solar. Batteries can play an important role here as well as they are a means to directly deliver and store electricity. Both trends reveal the criticality of effective storage of electricity by batteries. This then provides new opportunities for chemical industry to supply the materials and components that are needed for large scale manufacturing of batteries for electric vehicles as well as for grid scale storage. This presentation will describe recent trends in chemistry systems used in batteries for electric vehicles and those anticipated for grid scale storage. The needs for the associated materials can provide insights into new bulk chemicals that will be needed in large quantities.

Biography:

E. Takeuchi is a SUNY Distinguished Professor and Knapp Chair at Stony Brook University with a joint appointment at Brookhaven National Laboratory. She was previously at Greatbatch, Inc., where she developed the lithium/silver vanadium oxide battery to power implantable cardiac defibrillators. She is a member of National Academy of Engineering, the National Inventors Hall of Fame, the American Academy of Arts and Sciences, the National Academy of Innovation, and received the National Medal of Technology and Innovation, European Inventor Award, and the 2022 National Academy of Sciences Chemical Sciences Award. She is a Fellow of the ECS, AIMBE, and AAAS.

Title: Architected Catalytic Platforms Relevant to Alternative Fuels Production

Debra R. Rolison

U.S. Naval Research Laboratory, Washington, DC

Abstract Not Available!!!

Coupling Catalysis with Membrane for Energy and Environmental Applications

Sibudjing KAWI

National University of Singapore, Singapore

Abstract Not Available!!!

The charge transfer mechanism on a cobalt-polyoxometalate-TiO_2 photoanode for water oxidation in acid

Craig L. Hill[1]*, Fengyi Zhou[1], Xinlin Lu[1], Nandan Ghorai[1], Yiwei Yang[1], Yurii V. Geletii[1], Djamaladdin G. Musaev[1,2], Tianquan Lian[1]

[1]Department of Chemistry, Emory University, USA

[2]Emory Center for Scientific Computation, Emory University, Atlanta, GA USA

Abstract:

The oxygen evolution reaction (OER), a critical process in solar fuel production, continues to garner major research attention, with numerous (photo)electrocatalysts being identified and examined. However, achieving OER, especially under acidic conditions, is a challenge for metal oxide photoanodes, due to the sluggish four-hole oxidization process and the corrosive nature of an acidic environment. We report the fabrication of amorphous n-type TiO_2 photoelectrodes by initial treatment of the TiO_2 with cationic 3-aminopropyltrimethoxysilane (APS) ligand then with the molecular, well-characterized anionic $Na_8K_8[Co_9(H_2O)_6(OH)_3(HPO_4)_2(PW_9O_{34})_3]$ (**Co_9POM**) OER catalyst. Compared to the unmodified TiO_2, the functionalized TiO_2-APS-Co_9POM photoanode exhibits an approximately three-fold enhancement of OER photocurrent in a sulfate buffer at pH = 2. Spectroscopies (XPS, FTIR) show that the surface-bound **Co_9POM** retains its structural integrity throughout bulk electrolyses. We studied the catalytic effect of **Co_9POM** using open-circuit photovoltage measurements and transient absorption spectroscopy in both the visible and mid-IR ranges. Mechanistic investigations indicate that **Co_9POM** serves as an efficient OER catalyst, extracting photogenerated holes from TiO_2 on the picosecond timescale. Moreover, by shifting the TiO_2 band edge, the functionalized catalytic layer creates a favorable interfacial electric field, efficiently separating the photogenerated carriers and mitigating surface recombination.

Biography:

Craig L. Hill, Goodrich C. White Professor of Chemistry, studies catalysis, multifunctional nanomaterials, inorganic cluster compounds and solar fuel generation. He is a member of 4 academies/societies, has trained 160 PhDs and postdocs and has an H-index of 100.

Vanadium Compounds - Catalysis and Anticancer Activities

Debbie C. Crans

Colorado State University, Fort Collins, CO

Abstract Not Available!!!

Synthetic methanotrophic system to oxidize methane at ambient conditions into a growing polymer material

Michael S. Strano[1]*, Daniel James Lundberg[1], Jimin Kim[1]

[1]Massachusetts Institute of Technology, Cambridge, MA, USA

Abstract:

Methane is a critical fuel, chemical precursor, and potent greenhouse gas. Its production, transportation, and use result in its emission to the atmosphere, which induces ~30 times more warming than CO2 on a per-mass basis. Currently, there remains minimal understanding of efficient chemical methods for the conversion and/or valorization of methane streams—specifically under the conditions in which they are emitted i.e., low partial pressures and ambient temperatures. Here we report a synthetic methanotrophic system that is capable of oxidizing methane at ambient temperatures and pressures. Iron-modified ZSM-5 combined with the enzyme alcohol oxidase is found capable of driving methane oxidation continually and catalytically towards formaldehyde. We report to our knowledge the highest methane to formaldehyde selectivity to date for room temperature oxidation with peroxide—exceeding 90% under these conditions. We further show that the generated formaldehyde can be incorporated into a growing polymer through a reaction with urea, with a material growth rate exceeding 5.0 mg g_{cat} hr^{-1}, which meets and exceeds that of many cultured methanotrophic bacteria systems. The urea-formaldehyde polymer produced at room temperature was shown to be successfully incorporated into nanoparticle composites, with performance comparable to a commercially available urea-formaldehyde resin. This work presents a scalable and cost-effective route for methane oxidation at ambient conditions to produce a high-value polymer material. We believe this system will find direct and immediate use in the conversion and valorization of ambient methane emission streams.

Biography:

Professor Michael S. Strano is the Carbon P. Dubbs Professor of Chemical Engineering at the Massachusetts Institute of Technology. He received his BS from Polytechnic University in Brooklyn (NY) and PhD from the University of Delaware, both in Chemical Engineering. He was a postdoctoral research fellow at Rice University in the departments of Chemistry and Physics under the guidance of Nobel Laureate Richard E. Smalley. His research focuses on biomolecule/nanoparticle interactions and the surface chemistry of low dimensional systems, nano-electronics, nanoparticle separations, and applications of vibrational spectroscopy to nanotechnology.

Unlocking the Potential of Nitrous Oxide as a Chemical Feedstock- Functionalizing Hydrocarbons and Carbon Nucleophiles with N2O

Kenneth M. Nicholas

University of Oklahoma, Norman, OK

Abstract Not Available!!!

Janus structured nanomaterials: from design, fabrication to catalytic applications

Wei Wang

Aramco Americas: Aramco Research Center- Boston, Technology Square, Cambridge, MA , USA

Abstract:

As an emerging class of nanomaterials with asymmetric structures, the Janus nanomaterials have been successfully applied in many fields, including the growing field of catalysis in the past decade. In this review, we highlight the recent progress of Janus nanostructures from structural design, methods of fabrication and catalytic applications. Specifically, typical applications of Janus nanomaterials in micro/nano motors, interfacial catalysis, photocatalytic reactions, and catalytic conversion of materials for sustainable energy are summarized and discussed. A perspective of the potential industrial applications and possible further approach of Janus nanomaterials is also provided.

Biography:

Dr. Wei Wang, a Research Science Consultant, joined the Aramco Americas as a Founding Member of Aramco Research Center-Boston in 2012, and was a Staff Scientist at Oak Ridge National Laboratory (ORNL) in 2001-2012. His research focus is on application of advanced functional materials and nanotechnology for oilfields and sustainable energies. Wei earned his Ph.D. degree in Physical Chemistry at Chinese Academy of Sciences in 1993 and has authored >160 research papers (H-index 53), 5 book chapters, and 50+ US patents. Wei is a fellow of American Chemical Society (ACS), a fellow of Royal Chemical Society (RSC), and a Distinguished Lecturer of Society of Petroleum Society (SPE).

Amphiphilic catalysts for gas-liquid-solid reactions in non-aqueous foam

Marc Pera-Titus* and Kang Wang

Cardiff Catalysis Institute, School of Chemistry, Cardiff University, Cardiff, UK

Abstract:

Gas-liquid-solid (G-L-S) reactions are ubiquitous in the chemical industry. Conventional G-L-S reactors often suffer from mass transfer limitations due to their low G-L and L-S specific interface areas. High pressure is often required to boost the gas solubility in the liquid and promote mass transfer. A way out of this limitation is to design microbubbles and foams stabilised by catalytic particles in solvents as efficient G-L-S microreactors for conducting diffusion-free catalytic reactions at mild conditions.

Herein, we rationally designed amphiphilic ‘Janus’ particles with asymmetric wettability including oleophobic (or gas-philic) and oleophilic hemispheres, and catalytic moieties, to generate air-oil foams and conduct catalytic reactions at the gas-oil interface. Janus silica particles were prepared by sequential grafting of organosilanes in each hemisphere using the emulsion template method. Then, palladium nanoparticles were selectively deposited on each hemisphere by the sol-immobilization method. The particles were characterized by TGA, FTIR and $^{13}C/^{29}Si$ MAS NMR. The Pd-containing Janus particles could stabilize foams in aromatic solvents with a foam volume fraction up to 40% under magnetic stirring, and thus exhibit more than two-fold increase of catalytic activity compared to Pd-containing non-Janus particles, without generating foams, in the aerobic oxidation of aromatic alcohols in xylene. The Pd-containing Janus particles could be conveniently recycled by centrifugation for at least five consecutive runs keeping the foamability and catalytic activity.

Overall, this study supports the superior performance of Janus silica catalytic particles adsorbed at the gas-liquid interface for aerobic oxidation reactions.

Biography:

Marc Pera-Titus is chair of Sustainable Catalytic Chemistry at Cardiff University (UK). Marc received his PhD (2006) from University of Barcelona (Spain). In 2007, he joined Ircelyon/CNRS (France) as postdoc and was further appointed CNRS fellow in 2008. From 2011-2020, Marc was Deputy Director of the E2P2L CNRS-Solvay joint laboratory (Shanghai, China), merging academic and industrial reseach. Marc has published over 140 papers and invented 19 patents. Marc has received numerous awards, including the Silver and Gold Medals from the Chinese Academy of Inventions (2016, 2017), the DivCat award from the SCF (2017) and a ERC consolidator grant (2018).

Advanced Concepts for Ultra- High Conversion Efficiency of Solar Photons into Photovoltaics and Solar Fuels Based on Quantization Effects in Nanostructures and Molecular Singlet Fission

Arthur J. Nozik

Department of Chemistry and Renewable & Sustainable Energy Institute (RASEI)

University of Colorado, Boulder, CO and National Renewable Energy Laboratory (NREL)

Golden, CO

ABSTRACT:

In order to utilize solar power for the production of solar electricity and solar fuels on a global scale, it will be necessary to develop solar photon conversion systems that have an appropriate combination of high efficiency (delivered watts/m^2) and low capital cost ($/$m^2$). One potential, long-term approach to attain high conversion efficiencies above the well-known Shockley-Queisser thermodynamic limit of 33% is to utilize the unique properties of quantum dot/rod (QD/QR) nanostructures and Singlet Fission (SF) in molecular chromophores, to control the relaxation dynamics of photogenerated hot carriers and excited states in photoexcited molecules to produce either enhanced photocurrent through efficient photogenerated electron-hole pair (ie, exciton) multiplication or enhanced photopotential through hot electron transport and transfer processes. To achieve these desirable effects it is necessary to understand and control the dynamics of

SF and hot electron and hole cooling, charge transport, and interfacial charge transfer of the photogenerated carriers. These fundamental dynamics in various bulk and quantied nanoscale semiconductors and SF molecules have been studied for many years using various spectroscopies with fs to ns time resolution. The prediction that the generation of more than one electron-hole pair (which exist as excitons in size-quantized nanostructures and photoexcited molecules) per absorbed photon would be an efficient process in QDs,QRs, and SF molecules has been confirmed over the past years in different classes of materials, molecules, and their architectures. Very efficient and ultrafast multiple exciton generation (MEG), also called Carrier Multiplication (CM), and SF from absorbed single higher energy photons has been reported in many quantized semiconductors and molecules and associated solar photon conversion devices for solar electricity and solar fuels (e.g. H_2) production. Selected aspects of this work will be summarized and recent advances will be discussed, including the very remarkable and extremely large beneficial theoretical effects of combining MEG with solar concentration. The analogous MEG effect in SF molecules and its use in molecular-based solar cells will also be discussed.

Carbon-based metal-free electrocatalysts for Clean Energy and Environmental Remediation

Liming Dai

Australian Carbon Materials Centre

The ARC Centre of Excellence for Carbon Science and Innovation

University of New South Wales, Sydney, NSW, Australia

Abstract:

Since our discovery of the first carbon-based metal-free electrocatalyst (C-MFEC, *i.e.*, N-doped carbon nanotubes) for oxygen reduction in fuel cells in 2009, the field of C-MFEC has grown enormously. C-MFECs, as alternatives to noble metal-based electrocatalysts, have been widely demonstrated for efficient oxygen reduction, oxygen evolution, hydrogen evolution, carbon dioxide reduction, nitrogen reduction, and many other electrocatalytic reactions. Recent worldwide research effort has shown great potential for applications of C-MFECs in fuel cells for clean energy conversion, metal-air batteries for energy storage, water splitting for hydrogen fuel generation, and other electrochemical processes for value-added chemical production to reduce or even eliminate greenhouse emissions. Further research and development of C-MFECs could revolutionize clean energy and environmental remediation technologies. In this talk, I will summarize some of our work on the development of C-MFECs for clean energy and environmental remediation, along with an overview on recent advances, current challenges, and future perspectives in this exciting field.

Biography:

Liming Dai joined University of New South Wales (UNSW) in 2019 as an Australian Laureate Fellow (ARC), Scientia Professor and SHARP Professor at UNSW. He is also Director of the Australian Carbon Materials Centre and the ARC Centre of Excellence for Carbon Science and Innovation. Before joining UNSW, he spent 2 years in the Cavendish Laboratory (1990-1992) and 10 years with CSIRO (1992-2002). He was then an associate professor of polymer engineering at the University of Akron (2002-2004), the Wright Brothers Institute Endowed Chair Professor of Nanomaterials at the University of Dayton (2004-2009), and the Kent Hale Smith Professor in the Department of Macromolecular Science and Engineering at Case Western Reserve University (2009-2019).

Zero-Carbon Footprint in Waste-to-Energy: Integrating Chemical Looping Combustion with Red Mud Utilization for Efficient Sludge Treatment

Gursel Abbas[1]*, Ozge Yuksel Orhan[1]

[1]Hacettepe University, Turkey

Abstract:

Sewage sludge and red mud are examples of domestic and industrial wastes that adversely affect the environment. Due to their mass production and limited disposal options, addressing them in an environmentally appropriate manner has become an international concern. In chemical looping combustion (CLC), red mud containing high amounts of Fe_2O_3 and Al_2O_3 was used as an oxygen-carrier. Analysis has shown that the energy content of sewage sludge is equivalent to the coal used as an energy source. The microscopic shape, morphological structure, and properties of red mud heated up to 950°C have remained constant. The CO_2 selectivity in the flue gases resulting from CLC is 78%. Thus, the carbon capture process is made more efficient and easier. The most environmentally friendly and efficient methods have been applied in this facility to capture all the emitted carbon. Pre-heating of the water entering the process in the facility is done using solar energy, leading to an average annual fuel saving of 13.5%. Using the system's heat to dry the sewage sludge and red mud is another factor contributing to fuel savings. Additionally, in this project, the efficiency of the facility has been proven by performing SEM, XRD, XRF, higher heating value, moisture, ash, and volatility analyses of five different types of domestic sewage sludge, their ashes, and red mud. This research offers a unique method to the literature and industry for obtaining energy from domestic sewage sludge with use of red mud as an oxygen-carrier, following a zero-carbon footprint, renewable, and zero-waste approach.

Biography:

Gursel Abbas is a resilient Azerbaijani bachelors' chemical engineering student on the verge of completing his studies at Hacettepe University, Turkey. Despite severe injuries from an explosion accident, he excelled academically, securing the Erasmus+ Mobility scholarship three times and studying across Europe. His groundbreaking research on green energy from wastewater was recognized at TEKNOFEST. He co-authored a chapter in an Elsevier publication on CO_2 storage, highlighting his academic rigor. As a beneficiary of the U.S. Department of State's Ambassadors Fund for Summer Work Travel, he gained substantial international exposure. An avid traveler, Gursel Abbas has explored 23 countries, enhancing his global outlook.

Poster Presentations

PolyHIPE Composites For Latent Heat Storage: Flexibility And Enhanced Light To Heat Conversion

Presenter* and Co-author names (Jintao Lu[1*], Tao Zhang[2], Yan Zhao[3])

Affiliation ([1]Sun Yat-sen university, China; [2]Soochow University, China; [3]Soochow University, China)

Abstract:

Emulsion-templated, phase change material-encapsulated, monolithic polyHIPE composites are promising for latent heat storage, but their rigidity and low energy conversion limit the real applications. Here, we report the fabrication of phase-change material (octadecane, OD)-encapsulated polyHIPE composites with good flexibility and enhanced light/electro to heat conversion from surfactant-free emulsions. The composites were formed from interfacial cross-linking between isocynate and surface-modified carbon nanotubes and aminated cellulose nanocrystals which served as OD-in-water emulsion stabilizers. The resulting composites were flexible and exhibited robust compression (without failure even at 70% compressive strain), good encapsulation, high heat capacity (up to 220 J/g), and good reusability. Moreover, the composites exhibited enhanced light/electro to heat conversion efficiency (up to 90%), even at a low carbon nanotube content of around 0.1 wt %. These advantageous properties enabled the polyHIPE composites to be excellent candidates for latent heat storage and for light/electro to heat conversion.

Biography:

Jintao Lu, Doctoral students

Jintao Lu received his BS degree from at Hebei University of Science and Technology in 2019, and MS degree from Soochow University in 2022. He is a PhD candidate at Sun Yat-sen University since 2022, China. His research interest include the soft electronics and devices, energy conversion and storage, 2D materials and aerogel.

Mechanisms and Structural Characteristics in Photodegraded Material Carbon-Titania Hollow Nanostructures: A View by XAS

Yu-Wen Chen[1, 2], Wei-Hsiang Huang[2], Chin-Jung Lin[3], Yan-Gu Lin[2], Chung-Li Dong[4], Bing Joe Hwang[5], Wei-Nien Su[6], Shih-Yun Chen[1], Chi-Liang Chen[2*]

[1]Department of Materials Science and Engineering, National Taiwan University of Science and Technology (NTUST), Taipei, 106335 Taiwan

[2]National Synchrotron Radiation Research Center(NSRRC), Hsinchu, 30076 Taiwan

[3]Department of Environmental Engineering, National I-Lan University, Yilan, 260007 Taiwan

[4]Department of Physics, Tamkang University, Taipei, 25137 Taiwan

[5]Department of Chemical Engineering, National Taiwan University of Science and Technology (NTUST), Taipei, 106335 Taiwan

[6]Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology (NTUST), Taipei, 106335 Taiwan

Abstract:

The unique structure nanomaterials can be used as a photocatalyst to degrade the emerging water pollutant. We use carbon@titania hollow nanostructure for acetaminophen (Paracetamol) photocatalytic degradation in water. The photodegradation analysis studies have shown that the samples with different thicknesses of the shell and increased oxygen vacancies have improved the photocatalytic efficiency. X-ray absorption spectroscopy (XAS) Ti L-edge spectra discover critical charge transfer processes and holes that formed in the O 2p- Ti 3d hybridized bands significantly boost photodegradation ability under solar irradiation. The extended X-ray absorption fine structure (EXAFS) Ti K-edge results also showed that the amount of oxygen vacancies varied at changes in fabrication conditions, which has a significant effect on the electronic structure and a strong correlation to the local structural symmetry. In-situ XAS suggested a charge transfer at the interface between the shell and the presence of carbon under UV-visible illumination that enhances the photocatalytic activity. Enhanced performance of the hollow nanostructure can be attributed to the different shell surfaces and interfacial effects during the photodegradation reaction process.

Biography:

A beamline scientist at Taiwan Photon Source (TPS) 32A beamline (equipped with a diverse and promising beamline endstation) in NSRRC. Experienced synchrotron X-ray spectroscopy is adept in bringing forth expertise in the design, installation, measurement, analysis, and maintenance of optic systems—development of in-situ XAS and procedures. Manage independent physics science research projects, as well as collaborate as part of a research group team.

Synthesis and Characterization of Cobalt Complexes of Strong N-Donors with Sulfonamide Links

Nerissa A. Lewis[1]*, Luigi G. Marzilli[2], Yu-Jin Youn[1], Haley Willard[1], Kaitlyn Liu[1], and Frank R. Fronczek[2]

[1]Seattle Pacific University, USA; [2]Louisiana State University, USA

Abstract:

We are exploring methods to utilize strongly basic ligand analogues of 4-dimethylaminopyridine as a method for preparing bioconjugates that exploit coordination chemistry rather than mainly organic linking chemistry. The pyppzH (1-(4-pyridyl)piperazine) ligand has a basic pyridyl nitrogen for metal coordination and a secondary amine suitable for making sulfonamide links. Five new sulfonamide ligands, pyppzSO_2R (R = Me, 4-MeC_6H_5 = *p*-toluene, 3,5-$Me_2C_6H_3$ = 3,5-dimethylphenyl, Me_2Nnap = 5-(dimethylamino)naphthyl)), and $C_{10}H_8O$ (nap = 2-naphthalene)) were prepared. The reaction of the five pyppzSO_2R ligands with (Cl or CH_3)Co$(DH)_2$(py) (DH = monoanion of dimethylglyoxime) afforded the respective (Cl or CH_3)Co$(DH)_2$(pyppzSO_2R) complexes in good yields.

$_1$H NMR spectroscopic analysis (for all ligands and complexes) and single-crystal X-ray crystallographic data (for several ligands and complexes) established that the pyridyl group is bound to the cobalt metal center through the basic nitrogen atom in each case. ^{1}H NMR spectroscopic analysis also revealed a significant upfield shift in the pyridyl H2/6 signals, which is expected due to the magnetic anisotropy effect of the cobalt metal center. Molecules containing a sulfonamide group constitute a very important class of biologically active molecules with a wide variety of

applications. The use of this conjugation approach for the synthesis of novel pyppzSO_2R ligands and their cobalt complexes aids in developing new linkage chemistry applicable to the bioconjugation of useful molecules to potential targeting agents.

Biography:

Nerissa Lewis was born and raised on the beautiful island of Trinidad and Tobago. She earned her BS in chemistry at the University of the West Indies and then moved to the United States to pursue graduate studies. After completing her PhD in chemistry at Louisiana State University, she taught for four years at Walla Walla University, during which time she completed an MEd in curriculum and instruction, before joining Seattle Pacific University. Her research interest focuses on the synthesis and characterization of metal complexes with potential diagnostic and therapeutic activity for targeted delivery to tumor sites.

Dehydrogenation of Organic Molecules by Oxidation with Nitrous Oxide Using Ruthenium as Biomimetic Catalyst

Bruce A. L. Sacchelli

Universidade de Lisboa, Portugal

Abstract Not Available!!!

Layer-by-layer biocatalytic membranes for removal of micropollutants

Jakub Zdarta*, Teofil Jesionowski

Institute of Chemical Technology and Engineering, Faculty of Chemical Technology, Poznan University of Technology, Poznan, Poland

Abstract:

Enzymatic membrane reactors (EMRs) equipped with biocatalytic membranes are sustainable alternatives for removal of various micropollutants form water and wastewater under mild process conditions. Multifunctional biocatalytic membranes are considered as systems made of commercially available membrane modified by polyelectrolytes and immobilized enzymes, which are produced for complex treatment of water pollutants. Whereas multifunctionality of the produced membranes is related to the fact that these systems are capable of micropollutants removal via simultaneous catalytic conversion, adsorption and membrane rejection making remediation process more efficient.

In the presented study an attempts were made to obtain multifunctional biocatalytic multilayer membranes using polyelectrolyte layer-by-layer assembly with laccase immobilized in two ways: (i) between and (ii) into polyelectrolyte layers. For this purpose cationic poly-L-lysine and polyethylenimine as well as anionic poly(sodium 4-styrenesulfonate) polyelectrolytes were deposited onto commercial NP010 and UFX5 membranes to produce systems for removal of micropollutants. Based on preliminary study, four membranes with over 80% activity recovery, produced using polyethylenimine, were selected for degradation tests. Systems based on UFX5 membrane allowed over 60% of 17α-ethynylestradiol removal within 100 min, whereas NP010-based systems removed over 75% of estrogen within 150 min. In addition, around 70% removal of 17α-ethynylestradiol was possible from the solutions at concentration up to 0.5 mg/L and at pH ranging from 4 to 7. Finally, removal of around 70% of estrogen after 8 cycles of repeated use indicate high reusability potential of the systems and suggest their practical application.

Acknowledgements:

This work was supported by National Science Center Poland, as research project no. DEC 021/43/B/ST8/01854.

Biography:

Associate Professor Jakub Zdarta obtained a doctoral degree in 2017 in chemical sciences and become an associate professor in 2021. From 2018 he works in Institute of Chemical Technology and Engineering at Faculty of Chemical Technology, Poznan University of Technology. Author of over 110 scientific publications indexed by Thomson Reuters JCR and over 10 chapters in monographs. Principal or general investigator in a numerous of research projects financed by the National Science Center, NAWA and the Ministry of Science and Higher Education. The area of his research is focused on biotechnology, materials science, biocatalysis, environmental engineering, bioengineering, enzyme engineering, bioremediation and related fields.

Multifunctionality of Vanadium-based Catalysts with Tailored Properties and Activity for Selective Catalytic Reduction of Nox

Marcin Wysokowski

Poznan University of Technology, Poland

Abstract Not Available!!!

Absorption and Emission Characterization of Cerium(III) with 2-Pyrazinecarboxylate Ligands

Thomas Conroy[1]*, Kimberly Mullane[2]

West Chester University of Pennsylvania, USA

Abstract:

In 2015, an article was published in the *Journal of Photochemistry and Photobiology A: Chemistry* characterizing the absorption and emission of cerium(III) pyrazinoate, for use in various photocatalytic contexts, as a metal-to-ligand charge transfer. Notably, similar reported cerium complexes' fluorescence originate from f → d, LMCT, and ILCT transitions. By synthesizing and comparing cerium(III) pyrazinoate and lanthanum(III) pyrazinoate, this project aims to either confirm an unusual finding or gather evidence against the original paper's findings. Analytical techniques such as UV-vis spectroscopy, IR spectroscopy, $^{1}H/^{13}C$ NMR spectrometry, fluorescent emission spectroscopy, and single crystal X-ray crystallography were used to fully characterize the complexes in question. While there is evidence working against the paper's MLCT designation, further study is required to confirm the suspected f → d transition. Future research would include a dry synthesis of the compound to obtain a crystal structure of the complex without any water coordinated, allowing computational analysis to assist.

Biography:

I am a senior Chemistry major at West Chester University of Pennsylvania. I have been doing research with my professor, Dr. Mullane, for two semesters. Currently, I am participating in an internship for a company that does biochemistry research on neurodegenerative diseases. At home, I have two cats named Bo Bagel and Mayzie Marmalade who I love with all my heart.

Chemical Looping Combustion Integration for Efficient Waste Biomass Treatment

Gursel Abbas[1*], Ozge Yuksel Orhan[1]

[1]Department of Chemical Engineering, Hacettepe University, Turkiye

Abstract:

Conventional methods of wastewater treatment sludge disposal, such as land disposal, storage, and burial, pose financial and environmental challenges. This research introduces an innovative facility that not only addresses sludge disposal but also utilizes it for energy production, surpassing the efficiency of lignite-based energy production. The facility employs environmentally friendly approaches, aiming for a zero-carbon footprint. It uniquely combines the Chemical Looping Combustion (CLC) process, utilizing red mud from aluminum factories as an oxygen carrier, with solar pre-heating, efficient drying processes, and advanced particulate matter capture. The design, not found elsewhere, stands out internationally for its comprehensive and original approach. The study, based on Ankara Central Wastewater Treatment Plant sludge and Eti Aluminum's red mud, contributes a national perspective. Notably, the facility differs from others by producing water and carbon dioxide in the flue gas, ensuring high carbon capture selectivity. The use of solar energy and process heat for drying enhances efficiency, setting it apart from existing energy-producing facilities.

Biography:

Gursel Abbas is a resilient Azerbaijani recent bachelor's chemical engineering alumnus from Hacettepe University, Turkey. Despite suffering severe injuries from an explosion accident, he excelled academically, securing the Erasmus+ Mobility scholarship three times and studying across Europe. His groundbreaking research on green energy from wastewater was recognized at TEKNOFEST. He co-authored two book chapters in an Elsevier publication and an article in ACS. As a beneficiary of the U.S. Department of State's Ambassadors Fund for Summer Work Travel, he gained substantial international exposure. Starting in September 2024, Gursel will begin studying for his fully funded PhD degree in chemical engineering at the University of Wisconsin-Madison.

The End

Electrocatalytic carbon dioxide conversion to value-added multicarbon organics at high single product Faradaic efficiency and low over potential

Tao Xu

Northern Illinois University, DeKalb, Illinois, USA

Abstract:

The conversion of carbon dioxide (CO2) to value-added multi-carbon (with two or more than two C-C bonds) organic compounds by electrocatalytic reduction of CO2 provides a promising and value-added route to mitigate the greenhouse gas emission. Here, we present a family of carbon-supported transition and non-transition metals based electrocatalysts with varying sizes ranging from single atoms to few atom clusters that can electrochemically reduce CO2 to C2 and C3 liquid organic compounds with high single-product selectivity at relatively low potentials. The reaction mechanism is extensively studied by in situ synchrotron X-ray absorption techniques to identify the dynamic evolution of the catalytic center. It is stunning to reveal that atomically dispersed catalytic metal atoms aggregate to few-atom clusters under reductive potentials and depending on the redox potentials of the metals, oxygen atoms can also involve in the catalytic center. In addition, the supporting substrates exhibit a profound nano confinement effect that also impacts the reaction pathways towards C-C coupling. Our work renders atomistic and quantum mechanical level understanding in the reaction coordination for electrochemical CO2 reduction reaction to a versatility of value-added organic compounds. (Nature Energy, 2020, 5, 623-632)

Biography:

Dr. Tao Xu is the Distinguished Professor at Department of Chemistry, Northern Illinois University. Prof. Xu was awarded with National Science Foundation (NSF) CAREER Award in 2012, and NSF Special Creativity Award in 2022. He is also the recipient of two R&D 100 awards (2006, 2020) and is recognized as Researchers to Know 2020 by Illinois Science and Technology Coalition and the Innovator to Know 2023 by Illinois Innovation Network. Xu's group conducts fundamental studies on electron-driven and photon-driven interactions with a focuse on the design, synthesis, characterization and applications of novel energy and environment-related materials and structures.

Enhancing electrochemical CO_2 conversion by controlling electrocatalysts' structure

Thuy-Duong Nguyen-Phan[1,2]* and Douglas R. Kauffman[1]

[1]National Energy Technology Laboratory, Cochran Mill Road, Pittsburgh, PA , USA

[2]NETL Support Contractor, Cochran Mill Road, Pittsburgh, PA , USA

Abstract:

Electrochemical reduction of CO_2 (CO_2R) to valuable, carbon-neutral chemical feedstocks and storable fuels driven by renewable electricity has been recognized as one of the promising pathways to mitigate the greenhouse effect, reduce global demand for fossil fuels, achieve carbon neutrality, and create sustainable energy. Tremendous ongoing efforts have focused on controlling

the morphology, composition, structure, size, defects, etc. of the electrocatalysts to improve product selectivity, activity, and durability to approach the feasibility of practical applications (current density ~200 s mA/cm^2 and lifetime ~1000h+). The present talk will mainly discuss how the geometry and surface composition of novel copper and tin based catalysts would maximize the CO_2 conversion to carbon monoxide and liquid formic acid/formate in both common aqueous H-cell and electrolyzer configurations. Several spectroscopic, microscopic, and electrochemical characterization tools have been utilized to correlate the changes in the structural, physico-chemical, and electronic properties with the catalytic activity. Our work provides additional electrocatalyst design considerations for high performance CO_2 electrolysis.

Biography:

Dr. Thuy Duong Nguyen Phan is currently Senior Research Engineer of Battelle at U.S Department of Energy, National Energy Technology Laboratory (NETL). Dr. Nguyen Phan's research interests focus on functional materials for energy conversion (carbon capture and conversion, renewable chemicals/fuel production, hydrogen production/utilization), energy storage (battery, supercapacitor, oxygen storage), and environmental sustainability (wastewater/air/metal purification, indoor odor removal). She earned her Ph.D. in chemical engineering from University of Ulsan (South Korea) and then worked there as postdoctoral research fellow and research professor. Prior to working at NETL as contractor staff scientist, she worked as research associate at Brookhaven National Laboratory.

MgAl Layered Double Hydroxide as a Highly Efficient Bi-functional ElectroCatalyst for Green Hydrogen Generation

Rohit Srivastava* and Sneha Lavate

Catalysis & Hydrogen Research Lab, Department of Petroleum Engineering, School of Energy Technology, Pandit Deendayal Energy University, India

Abstract:

Green hydrogen production from water electrolysis has become a potential technology for replacing non-renewable exhaustible energy resources. The utilization of low cost, bifunctional catalysts and renewable energy sources for electrolysis of water helps to reduce the energy consumption and produce high yield of green hydrogen (H2). This research paper describe the facile synthesis of Mg-Al Layered Double Hydroxide (LDH) electro-catalyst through hydrothermal method for green H2 generation. The phase identification of crystalline material can be analyzed by using X-ray diffraction technique, whereas surface area of synthesized LDH electro catalyst was determined by using BET experimental data. The surface morphological structure of LDH catalyst was observed by using SEM images. From the electrochemical measurement data it was found that the synthesized electro catalyst possess a cathodic current density of 10 mA/cm2 at 1.987 V and anodic current density of 10 mA/cm2 at 1.378 V and low Tafel slope which indicates the good electrochemical stability of Mg-Al LDH in basic medium. The synthesized electrocatalyst can be further use for the development of alkaline electrolyzer in order to produce the green hydrogen at larger scale. Biography: Dr. Rohit Srivastava earnned his Ph.D. degree from Birla Institute of Technology, Mesra, Ranchi, India, in 2015. He spent more than 1 year as Dr. D S Kothari Postdoctoral Fellow at the Department of Inorganic and Physical Chemistry, IISc, Bangalore, India. Afterwards he worked as a Post-doctoral at Harvard University Cambridge USA, from year 2016

to 2018. Dr. Srivastava published more than 30 research paper in high impact journal and wrote 5 international books. At present Dr. Srivastava holds the position of Senior Assistant Professor at Department of Petroleum Engineering, Pandit Deendayal Energy University, Gandhinagar Gujarat India, and working in the area of green Hydrogen and CO2 reduction into green fuels. His current thrust areas of research include Green Hydrogen, Electro/photo-chemical Technology, Energy Storage & Conversion and origin of life.

Controlled Aqueous-phase Synthesis of Surfactant-free Porous Pd/M (M = Au, Cu, Mn) Sponge-like Nanocrystals for Boosted Alkaline Ethanol Oxidation

Aboubakr M. Abdullah[1]*, Adewale K. Ipadeola[1,2], Belal Salah[1,2], Ahmed Abdelgawad[2], and Kamel Eid[2]

[1]Center for Advanced Materials, Qatar University, Doha, Qatar.

[2]Gas Processing Center (GPC), College of Engineering, Qatar University, Doha, Qatar.

Abstract:

Electrochemical ethanol oxidation reaction (EOR) is a crucial parameter in the fabrication of reliable alcohol-based fuel cells, however, its sluggishness necessitates the search for highly active and durable electrocatalysts. The engineering of Pd-based alloys (i.e., PdM) with distinct physicochemical merits is effective for improved EOR. Herein, a simple, aqueous-phase, one-step, and ultrafast approach for the preparation of surfactant-free porous PdM (M = Cu, Au, and Mn) nanocrystals with well-controlled spongy-like morphology and compositions. The electronic feature in PdM nanocrystals and the alloying effect on the alkaline EOR are thoroughly probed. Interestingly, M metals integration into the Pd lattice led to an upshifted d-band center to boost the EOR activity and durability significantly. Thus, the EOR mass activity of PdCu was 1.83, 3.09, 4.51, and 53.90 times higher than those of AuPd, PdMn, Pd and Pd/C, respectively, besides significant durability after 1000 cycles. This was ascribed to the porous two-dimensional structure, low synergy, higher interfacial contact and surface area of PdCu, besides the increased oxophilicity of Cu that enables activation/dissociation of H_2O to generate ^{-}OH species required for fast EOR. Electrochemical impedance spectroscopy (EIS) revealed better electrolyte/electrode interfacial contact and lower charge transfer resistance on PdCu. Also, the EOR activity of PdCu sponge-like nanocrystals was superior to all previously reported Pd-based alloys for the EOR. This study revealed that low synergy in PdM catalysts is preferred for boosted EOR performance and durability, which could help to direct the surface architectures of Pd-based alloys to optimum EOR in alcohol-based fuel cells.

Biography:

Prof. Aboubakr Abdullah has 30 years of experience in academia and industry. He published over 200 peer-reviewed articles/conference proceedings and 7 USA-granted patents. He earned his Ph.D. (2003) from the Pennsylvania State University. Since he joined Qatar University (2012), he has managed more than ten research mega-projects funded by different agencies (Qatar National Research Fund (QNRF), Qatar University, Hydro/Qatalum, Qatar Power (QP) and Qatar Shell (QS)). Also, he offered consultations for different companies (Qatar Gas, Qatalum, Qatar Electricity and Water Company (QEWC), and Kahramaa). In 2020, he won the Qatar University Research Excellence Award – “Science and Engineering Path“

Electrocatalytic Successor Technologies for Chemical Manufacturing

Astrid Mueller

University of Rochester, Rochester, NY

Abstract Not Available!!!

Photocatalytic Oxidation of VOCs at High Destruction and Removal Efficiency

Melissa A. Petruska[1]*, Robert T. Henderson[1], Mostafa Dehghanizadeh[1], Thomas J. Spoonmore[1]

[1]Sonata Scientific LLC, USA

Abstract:

Despite decades of research in photocatalysis, adoption of photocatalytic air purification is not widespread. One barrier had been the possibility of incomplete oxidation, which may lead to the release of chemical by-products. A second hurdle to overcome is low volatile organic compound (VOC) destruction and removal efficiency (DRE), largely a result of poor mass transfer and insufficient light interaction with the photoactive species. Sonata Scientific has developed a novel system that integrates a highly engineered photocatalyst in a fluidized-bed photoreactor, which maximizes mass transfer and light coupling to the photocatalyst. This approach enables an unprecedented 99+% DRE for a wide variety of VOCs and organic gases, including formaldehyde and ethylene oxide, without release of measurable by-products, even at concentrations of 1 ppm or lower where other abatement strategies are energy intensive and fall short. This catalyst/system design is differentiated from current photocatalytic approaches and enables its application in a range of highly demanding industrial applications. Test data collected for different challenge species under a variety of real-world operating conditions will be presented.

Biography:

Dr. Melissa Petruska is Vice President of Product Development at Sonata Scientific LLC, an early-stage company that is transforming its materials chemistry and systems innovations into practical products to improve living and working environments. She has extensive experience in developing innovative technology and products for a variety of fluid purification and gas and energy storage applications. Currently she leads the development of Sonata Scientific's air purification technology platform. She has authored more than 30 technical publications and is an inventor on 16 patents. Dr. Petruska was also recognized as a 2020 Connecticut Women of Innovation finalist.

Mechanisms Guiding Photocatalytic Csp2−Csp3 Cross-Coupling

Hannah Sayre*

Northeastern University USA

Abstract:

Photocatalysis with an Ir(III) photosensitizer and Ni(II) organometallic catalyst enables Csp2 − Csp3 cross-coupling. Critical Ni(II) intermediates were identified during mechanistic investigation. Time-resolved spectroscopy, pulse radiolysis, and EPR experiments reveal dominant energy

transfer mechanisms in three Csp2 −Csp3 cross-coupling reactions.

Biography:

Hannah Sayre is a photochemist researching light-activated chemistry. She earned a MS from Virginia Tech where she studied supramolecular photocatalysts with Karen Brewer in 2015. She completed her PhD in 2018 at The Ohio State University while developing red light-activated dirhodium catalysis with Claudia Turro. Under the direction of Gregory Scholes at Princeton University, she was the lead distinguished postdoctoral researcher for Bio-Inspired LightEscalated Chemistry (BioLEC), an Energy Frontier Research Center funded by the U.S. Department of Energy. She has been a faculty member at Northeastern University since 2021.

Low Temperature Fuel Cell at Direct-Reformate CO Concentrations

Anastasios P. Angelopoulos [1*] and Pranjul Dubey[1]

[1]University of Cincinnati, Department of Chemical and Environmental Engineering

Abstract:

Low temperature proton exchange membrane fuel cells (LT-PEMFC) are technologically proven sources of clean, sustainable, and environmentally friendly alternatives to petroleum for light duty and automotive applications. Unfortunately, the absence of a widespread hydrogen fuel distribution network represents a significant obstacle to the introduction of the kind of economies of scale needed to make PEMFC technology cost competitive. On -board reforming has been a long sought after goal as a means of overcoming this obstacle through utilization of alternate interim sources of hydrogen ranging from biofuels to petroleum or industrial waste effluent (e.g., carbonization byproducts). Unfortunately, even with the best available electrocatalysts such as PtRu, ultra-high purity hydrogen (H_2>99.9%) is needed to prevent loss of power due to the irreversible adsorption (poisoning) of CO at the catalytically active sites. Depending on the fuel source, typical CO concentration in reformate can range from 1% up to 10%. We will here present bench-scale electroanalytical data for novel, self-supported PtBi nanoplatelets of ~5 nm thickness which exhibit substantially reduced onset potential and faster kinetics for CO oxidation relative to PtRu. Such behavior is found to yield steady-state power generation from 5 cm^2 PEMFC's operating at temperatures as low as 60^{o}C with hydrogen fuel containing 1% CO at 0.2 A/cm^2. Unlike the oscillatory behavior observed at 0.1% CO with PtRu electrocatalyst, steady-state power is reached at 30% that of pure hydrogen with 3% CO oxidation. There is currently no competing LT-PEMFC electrocatalyst that can achieve this performance.

Biography:

Dr. Anastasios P. Angelopoulos is Professor and Head of the Department of Chemical and Environmental Engineering at the University of Cincinnati (UC). His research is focused on development of sustainable synthesis methods for fuel cell electrocatalysts, particularly for direct-reformate use. Prior to joining UC, Dr. Angelopoulos was Senior Materials Scientist at the General Motors Fuel Cell Research and Development Center in Honeoye Falls, NY., where he directed the failure analysis of proton exchange membrane (PEM) fuel cell components. He holds a total of 16 issued patents.

Visible-light Induced Oxygenation of Aromatic Compounds Using Photoredox Catalysts

Kei Ohkubo[1,2*]

[1]Institute for Advanced Co-Creation Studies, Osaka University, 1-6 Yamada-oka, Suita, Osaka 565-0871, Japan

[2]Institute for Open and Transdisciplinary Research Initiatives, Osaka University, 1-6 Yamada-oka, Suita, Osaka 565-0871, Japan

Abstract:

Photocatalytic oxygenation of benzene occurs in an oxygen-saturated acetonitrile solution containing acridnium ion or quinolinium ion derivatives as a photoredox catalyst, benzene and water under light irradiation to yield phenol and hydrogen peroxide selectively. The benzene radical cation, which is formed by photoinduced one-electron oxidation of benzene with the excited state of catalyst, reacts with H2O to yield phenol. Photocatalytic oxygenation of benzene with oxygen occurs under photoirradiation of an acetonitrile solution of 3-cyano-1-methylquinolinium perchlorate (QuCN+ ClO4 –) in an oxygensaturated acetonitrile (MeCN) containing benzene and H2O with a xenon lamp (500 W) attached with a color-cut glass filter. The selectivity of formation of phenol was 98% with 16% quantum yield after 1 h irradiation, and then 51% of phenol yield after 5 h irradiation. The photocatalytic turnover number (TON) was 7.5. This is the first example of photocatalytic oxygenation of benzene to phenol in a homogeneous system. A preparative gram-scale photocatalytic reaction with benzene (2.3 g, 29 mmol) and QuCN+ (210 mg, 0.8 mmol) in MeCN (200 mL) for 48 h was also examined to afford phenol (1.1 g, 12 mmol) as 41% yield.

Biography:

Dr. Kei Ohkubo, Chemistry Doctor (Ph.D. Engineering), now is a Professor of Chemistry of Institute for Advanced Co-Creation Studies and Institute for Open and Transdisciplinary Research Initiatives, Osaka University, Japan. He earned his Ph.D. degree from Graduate School of Engineering, Osaka University in 2001. He was working as a JSPS fellow and a JST research fellow at Osaka University (2001-2005), a designated associate professor in Osaka University (2005-2014) and a specially appointed professor at Osaka University (2014-2017). He has been a full professor at Osaka University since 2017.

Roles of Photocatalysis in the Origin and Evolution of Life on Early Earth: The First Organisms on Earth were Possibly Phototrophic Methanotrophs and Cyanobacteria that Evolved on Mineral Surfaces Under a Methane-Rich Atmosphere

Hiroshi Ohmoto

Abstract Not Available!!!

Photocatalytic Characteristics of TiO$_2$/g-C$_3$N$_4$ Supported on the Calsium Aluminate Long-lasting Phosphor

Jung-Sik kim*,_ Qiushi Xu, Shielah Mavengere

Dept. of Materials Science and Engineering, University of Seoul, Seoul, Korea

Abstract:

Triply doped $CaAl_2O_4:Eu^{2+}$, Nd^{3+}, and Gd^{3+} phosphors were synthesized using a solid-state method at 1300 °C and coupled with TiO_2/g-C_3N_4. The effects of the Gd^{3+} concentration as a codopant on the emission intensity and afterglow performance of the phosphors were investigated. The characterization of $CaAl_2O_4:Eu^{2+}$, Nd^{3+}, and Gd^{3+} was performed via X-ray diffraction, scanning electron microscopy, UV-Vis absorption spectroscopy, and energy-dispersive spectroscopy. Fluorescence spectroscopy was performed to evaluate the excitation, emission, and afterglow-decay properties of the synthesized phosphor. The Gd^{3+}-co-doped $CaAl_2O_4:Eu^{2+}$, Nd^{3+} phosphor exhibited enhanced luminescence properties in relation to a commercial $CaAl_2O_4:Eu^{2+}$, Nd^{3+} phosphor. In addition, outstanding photocatalytic efficiencies were observed for the Gd^{3+}-co-doped $CaAl_2O_4:Eu^{2+}$, Nd^{3+} phosphor/TiO_2/g-C_3N_4 composite in relation to those for the non-Gd^{3+} samples under UV-light illumination. Alternatively, Gd^{3+}-doped and undoped $CaAl_2O_4:Eu^{2+}$, Nd^{3+}/TiO_2/g-C_3N_4 exhibited similar photocatalytic efficiencies under visible-light illumination

Biography:

Affiliation:

Department of Materials Science and Engineering, University of Seoul, Republic of Korea

Position: Professor

Education:

1987-1992, MS, Ph.D. : Dept. of Materials Engineering, Purdue University, USA

Research interests:

Photocatalysts, Chemical Sensors

The Use of Asymmetric Catalysis for the De Novo Synthesis of Oligosaccharide

George A. O'Doherty

Abstract Not Available!!!

Mechanistic Insights Facilitate the Development of New Bond Forming Processes

Andy A. Thomas

Department of Chemistry, Texas A&M University, USA

Abstract:

Organolithium reagents have been shown to be powerful tools in asymmetric synthesis, from the desymmetrization of meso epoxides to ortho-substitution reactions. Despite these achievements, the ability to activate positions without the aid of directing groups in saturated systems appears to have reached an evolutionary dead end. Using our rapid injection NMR technique, we have determined that the aggregate structure of organolithium reagents can be altered with phosphoramides allowing for unique positions within saturated oxygen heterocycles to be activated. Guided by our mechanistic insights we have developed a simple γ–deprotonation

substitution protocol to access chromane products. This strategy could be applied to a variety of terminal bromides that contained various functional groups as well as substituted chromane substrates in good to excellent yields.

Biography:

Dr. Andy Thomas is currently an assistant professor at Texas A&M University. He received both his B.S. and M.S. degrees in chemistry from the University of North Carolina at Charlotte. In 2011 he moved to UIUC to begin his Ph.D. with Prof. Scott Denmark. Upon completion of his Ph.D. in 2017 he began his NIH postdoctoral fellowship at MIT with Prof. Stephen Buchwald. In the Fall of 2020 Andy joined the chemistry faculty at Texas A&M University as an assistant professor. His research group focuses on developing new synthetic methods by investigating the chemical reactivity of highly reactive intermediates.

Optical Spectra and Emission Properties of Early Transition Metals (Zr, Hf)

Kimberly C. Mullane*, Margaret Page, Nelson Pineda, Ezinne Ottih

West Chester University, USA

Abstract:

Photoredox catalysis has been used in recent years to perform otherwise challenging organic transformations, such as dehalogenation, cross coupling, and C–H bond oxidation reactions. While the most well-known photocatalyst, Ru(bipy)3, undergoes a metal-to-ligand charge-transfer (MLCT) in its photochemical mechanism, recent examples of zirconium and cerium photocatalysts often exhibit ligandto-metal charge-transfers (LMCT) in their catalytic cycles. My lab is working to study the light absorption and emission forzirconium and hafnium complexesfor application in photochemical separation. Although zirconium and hafnium metals are notoriously difficult to separate, some related complexes absorb different wavelengths of light. We aim to use differences in zirconium and hafnium excitation with light to selectively photoreduce and separate the two metals. We have synthesized trifluoroacetylacetonate complexes of zirconium and hafnium and observed a solvent–dependent difference in molar extinction coefficients. Additionally, we have synthesized and characterized highly–conjugated salen–type complexes of zirconium and hafnium. These complexes absorb visible light and are studying their photochemistry and redox properties.

Biography:

Kim completed her undergraduate degree in Chemistry at Bryn Mawr College and went on to complete her PhD in Inorganic Chemistry at the University of Pennsylvania in the lab of Prof. Eric Schelter where she studied the reactivity and electronic structures of uranium complexes with nitrogen and oxygen donors in axial symmetries. During her time at Penn her work was acknowledged by the Department of Energy for Innovations in Fuel Cycle Research. Currently, she is an Assistant Professor at West Chester University where she and her students are working on synthesis of Group IV and lanthanide complexes.

Electrochemical Growth and Restructuring of Cu Nanoparticles for Steering the Selectivity of Electrocatalytic CO2 Reduction

Joseph S. DuChene*

Department of Chemistry, University of Massachusetts Amherst

Abstract:

The electrocatalytic reduction of CO2 into value-added chemicals is commonly performed with catalysts composed of Cu due to its propensity for producing C2+ products like ethylene and ethanol. While promising, the reaction is known to suffer from poor selectivity. Several studies have shown that the surface facets of Cu catalysts play an important role in dictating the distribution of CO2 reduction products, yet the dynamic nature of Cu surfaces leads to significant surface reconstructions that alter the catalyst selectivity over the course of the reaction. The factors governing the evolution of Cu surfaces during CO2 reduction must be fully understood to enable control over these processes at the atomic level. Here, we discuss our efforts towards controlling the surface facets of Cu electrocatalysts via electrochemical treatments for steering the selectivity of electrocatalytic CO2 reduction. Using both polycrystalline Cu foils and shape-controlled Cu or Cu2O nanoparticles, we will show how the applied potential and chemical composition of the growth solution can be manipulated to tailor the surface facets of Cu electrocatalysts. Finally, we will present the results of electrocatalytic CO2 reduction with these nanostructured Cu catalysts and highlight opportunities for using simple electrochemical techniques to tailor the surface facets of electrocatalysts at the nanoscale for the selective production of chemical fuels. We anticipate that these studies will lead to new strategies for maintaining preferred surface facets during the electrocatalytic reaction or inform simple electrochemical methods for reconstruction of the catalyst surface to recover the initial reaction selectivity.

Biography:

Joe DuChene is an Assistant Professor of Chemistry at UMass – Amherst, where his group designs and creates nanostructured catalysts for sustainably synthesizing fuels and chemicals from readily abundant pollutants. Prior to joining UMass Amherst, Joe was a postdoctoral scholar in the group of Harry Atwater at Caltech, where he conducted fundamental studies of plasmonic hot carriers in metal nanostructures and pioneered new plasmonic devices for enhancing the selectivity of photoelectrochemical CO2 conversion. Joe obtained his Ph.D. in Physical Chemistry from the University of Florida working with Professor David Wei on the development of plasmonic photoelectrochemical cells for solar-to-fuel energy conversion.

Synthesis of Multi-metallic Nanocatalysts Using a Dendrimer Reactor

Kimihisa YAMAMOTO

Tokyo Institute of Technology, Nagatsuta, Yokohama , 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 polyphenyl-azomethine 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.

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A Solvent/Solute Model for Carbon Nanotube Growth

Mark A. Banash*

President and Chief Scientist (Neotericon LLC, USA)

Abstract:

The term “catalyst” within the context of large-scale production of carbon nanomaterials (CNTs) may be a misnomer. The growth of CNTs using metal nanoparticles in a flow reactor is perhaps better understood not by the defined mechanisms and processes of catalysis but instead by a much simpler solvent/solute process involving feedstock and adjuvants dissolving as free atoms in a liquid with assembly dictated by surface energy effects. This would explain why some species such as sulfur seem to promote the reaction instead of acting as a poison.

Starting with Sieverts’ Law the thermodynamics of such a process are presented to provide insight into how CNT synthesis can be improved. Data from experiments done to explore the resulting model are also presented, including the effects of alternate metal sources. Electron microscopy will reveal the associated effects on the morphology of the CNTs made, and thermogravimetric

analysis will show elementary changes in purity and the types of surfaces produced.

Biography:

Mark Banash is President and Chief Scientist at Neotericon, LLC, a nanotechnology/nanomaterials consultancy. Prior to this as VP-Chief Scientist at Nanocomp Technologies Inc. (now Huntsman) he was responsible for all aspects of carbon nanomaterial production from understanding synthesis to nanometrology to finished product testing. Before Nanocomp he was Director of Production at Zyvex where he oversaw the creation of their carbon nanotube thermoset and thermoplastic resins. His BA in Chemistry is from the University of Pennsylvania and his PhD in Chemistry is from Princeton. He also serves on the ISO TAG on nanomaterials.

Catalysts for Decarbonization: What Do We Need To Achieve Net Zero 2050

Magda H. Barecka

Northeastern University, Boston, MA

Abstract Not Available!!!

Downfolding in Atomic and Molecular Physics

Mark R. Hoffmann* and Tsednee Tsogbayar

University of North Dakota, USA

Abstract:

Quantum Chemistry is traditionally done by assuming a form for the wavefunction and optimizing parameters. Alternatively, one could ask the question whether the Hamiltonian operator itself could be modified. One could do this in an ad hoc manner, as is commonly done (i.e. for semi-empirical methods), or one could seek a systematic method for this downfolding. We are exploring a method of downfolding introduced by Wilson and by Wegner, which has proven useful in nuclear physics by Bogner and coworkers. Formally, it is an Effective Field Theory built along Renormalization Group ideas. Besides discussing the mathematical model, examples from atomic and molecular physics will be given.

Biography:

Hoffmann has developed a number of electronic structure methods, most notably Unitary Couple Cluster and GVVPT2. Tsogbayar is currently a posdoc in Hoffmann's group.

Solar water splitting using epitaxial thin films photoanodes

A. Barbier[1]*, A Derj[1], C. Blaess[1], H. Lin[1], M. Rioult[1], S. Datta[1], D. Stanescu[1], S. Stanescu[2], G. Creutzer[1], H. Magnan[1], S. Matzen[3], J.-B. Moussy[1], C. Mocuta[2], F. Charra[1], M. Silly[2], R. Belkhou[2], P. Le Fèvre[2], J. Leroy[4], F. Maccherozzi[5]

[1]CEA/Saclay, Service de Physique de l'Etat Condensé, France;

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[4]IRAMIS/NIMBE Université Paris –Saclay, CEA, CNRS, France;
[5]Diamond Light Source, Oxforshire, United Kingdom.

Abstract:

The development of green and sustainable chemical processes represents a major challenge within chemistry. Oxides and oxynitrides offer a very wide range of properties allowing for a multitude of applications and many have the required chemical stability for photocatalytic applications such as solar water splitting and/or CO2 reduction. However, their performance is often deceiving due to unfavorable band gap (values and positioning with respect to the redox levels) or charge recombination. We have been developing model thin films for solar water splitting prepared by plasma-assisted molecular beam epitaxy for several years, in order to understand the relevant parameters to improve the performance of photoanodes. We studied the effectiveness of doping (Ti and O vacancies) in Fe2O3, the role of electric polarization in BaTiO3 and more recently the impact of nitrogen doping in BaTiO3. We used an original approach consisting in using the substrate as the oxygen supplier and atomic nitrogen plasma to incorporate substitutional N atoms into the perovskite lattice. The layers were characterized by *in situ* by high-energy electron diffraction, Auger and photoemission spectroscopies, and *ex situ* by synchrotron radiation X-ray diffraction and spectroscopies, optical absorbance, ferroelectric behavior as well as photoelectrochemical response. Each system allowed pinpointing the role of specific parameter in the improvement of the photoelectrochemical activity of the film.

Biography:

Dr. Antoine Barbier is a research director and “expert senior” scientist at CEA where he is a specialist for the field of synchrotron radiation and oxides thin films studies. He holds a PhD and HDR in Solid State Physics from university of Strasbourg. With a strong background in surface physics/chemistry and magnetic thin films, he joined CEA in 1994 where he studied polar oxide surface structures. His research interests moved to oxides thin films and heterostructures. Currently, his researches focus on oxide thin films for spintronics and solar water-splitting applications using a large panel of laboratory and synchrotron radiation techniques.

Recent Advances in Selective Catalytic Reduction of NOx at Low Temperature

Yuegang Zuo*†, Chengjun Wang† and Chen-lu Yang‡

†Department of Chemistry and Biochemistry and ‡Advanced Technology and Manufacturing Center, University of Massachusetts Dartmouth,North Dartmouth, MA

Abstract:

Decomposition of NO_x into N_2 and O_2, a thermodynamically favorable reaction at low temperature, is desirable. However, the reaction is very slow and sufficiently active catalysts have not been discovered. As a result, various reductants, such as CO and CH_4, have been tested to reduce NO_x into N_2. But these reactions require the catalysts made of noble metals such as Pt, Pd, and Rh, and high cost of facilities, and still suffer from the low removal efficiencies at low temperature. In this presentation, we will report on the recent developments in selective catalytic reduction (SCR) for eliminating NO_x from stationary sources such as power plants, and automotive exhausts. Such technique offers the advantages of low cost, high selectivity and the possibility for converting

the noxious gas to one or more innocuous substances such as nitrogen gas and water, which are free of disposal problems. A novel copper-based catalyst has been synthesized in our research laboratory and evaluated for its efficiency on the selective catalytic reduction of nitric oxide (NO) using ammonia (NH_3) as a reductant in the temperature range of 50~500 °C. The catalyst shows high activity for NO conversion (90%) with a NH_3/NO ratio of about 1 in the presence of O_2 (~ 3% v/v) at a temperature of 200 °C, indicating that the developed Cu-based catalyst is very promising for the elimination of NO using NH_3 as a reductant in flue gases. Details on the SCR of NO and the mechanisms involved will be discussed at the presentation.

Biography:

Yuegang Zuo is currently a Chancellor Professor at Department of Chemistry and Biochemistry, University of Massachusetts Dartmouth. He is also a Full Professor in marine sciences at the School of Marine Science and Technology, University of Massachusetts. He received his Ph.D. in environmental science from Swiss Federal Institute of Technology Zurich in 1992. Most of his recent research has focused on emerging organic and inorganic pollutants and their occurrence, sources, distribution, transportation and fate in the biochemosphere. He has published over 90 peer-reviewed papers in prestigious international scientific journals such as Science, Environmental Science and Technology, and JAFC.

Multifunctional Catalysts for Selective Hydrocracking of Polypropylene to liquid hydrocarbons in jet fuel range under Mild Condition

Gillian Goh1* , Wei Jie Yap1 , Jennet Li Ying Ong1 , Man Fai Ng2 , Teck Leong Tan2 , Xian Jun Loh1,3 and Lili Zhang1

[1]Institute of Sustainability for Chemicals, Energy and Environment (ISCE2), Agency for Science, Technology and Research (A*STAR), 1 Pesek Rd, Singapore 627833, Republic of Singapore

[2]Institute of High Performance Computing (IHPC), Agency for Science, Technology

Abstract:

and Research (A*STAR), 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632, Republic of Singapore 3 Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR), A∗STAR, 2 Fusionopolis Way, Singapore 138634, Singapore

The widespread applications of polypropylene (PP) had resulted in a rapid generation of its waste1 which should be addressed to reduce carbon emissions by incineration and to transform PP waste into valuable products in a circular economy. Currently, researchers had focused their efforts on the catalytic depolymerization of plastic waste to generate the value-added hydrocarbons. It is noteworthy that while the reported reaction conditions were mild2-4 , the conversion and selectivity towards liquid hydrocarbons (C8-16) were moderate. Much harsher conditions, either at high pressure and long reaction times or with additives, were required to achieve an improved yield. Therefore, a highly selective and efficient pathway towards saturated hydrocarbons in the range of C8-16 for the use of jet fuel under mild conditions is desirable. Here, we report the multifunctional heterogeneous catalyst system (i.e., XYO3/meso Al-Si) 5,6 that is highly selective towards the production of liquid hydrocarbons (C8-16) through hydrocracking of PP at mild conditions in the absence of solvent to achieve a high yield and selectivity of 78 % and 81%. Several features such as appropriate amount of strong hydrogenating metal X and the strong

Brønsted acidity of the XYO3/meso Al-Si catalyst system come together to result in an optimized processive multifunctional catalytic hydrocracking of PP to afford desired C8-16 hydrocarbons in a high yield and selectivity.

Biography:

Gillian Goh is currently a scientist at Agency for Science, Technology and Research (A*STAR), Institute of Sustainability for chemicals, energy, and environment (ISCE2), Catalysis and Green Process Engineering since 2021. She was working as a research fellow at Institute of Chemical and Engineering Sciences (ICES) from 2020-2021. She specializes in low carbon technologies for waste upcycling to carbon neutral fuels contributing to the Zero-waste masterplan and the National CO2 emissions target. She graduated from Nanyang Technological University with a 2 nd Uppers honor (Bachelor), specialization in medicinal chemistry (2016) and a Doctor of Philosophy in Chemistry and Biological Chemistry (2020).

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Enhancing ethylene activation through substituted polyoxometalates enables electrified synthesis of ethylene glycol

Jiaqi Yu[1,*] and Edward Hartley Sargent[1]

[1]Northwestern University, USA

Abstract:

Organic oxidation reactions (OOR), such as the conversion of ethylene to epoxides and diols, have an average carbon intensity of 2.6 and 1.9 ton-CO_2e/ton-product, and annual global carbon emissions of 78 and 55 million ton-CO_2e. Electrified OOR (eOOR) is a promising approach to reduce energy intensity and carbon emissions; however, direct eOOR suffers from low reaction rates due to low mass transfer of insoluble olefins. Halide-mediated systems have shown improvements in eOOR rates, but so far these have exhibited high voltages that lead to low energy efficiencies and limited technoeconomic potential. Here we pursued the design of new mediators that promote eOOR reactions, finding that polyoxometalates, comprising electron-withdrawing oxyanions such as W(VI) and Mo(VI), both oxidize and stabilize nucleophilic alkenes. A substituted polyoxometalate achieves 82% faradaic efficiency in ethylene oxidation to ethylene glycol (EG), with a full cell voltage of 2.3 V at 100 mA/cm^2. The low full cell voltage leads to <~ 9 GJ/(1 ton EG + 0.04 ton H_2) energy consumption from this electrified route at 100 mA/cm^2; this compared to 29 GJ/ton for the industrially-practiced thermocatalytic route and 12 GJ/ton for the best previously-reported Cl--mediated ethylene oxide production route. Mechanistic studies indicate that POM plays a dual shuttle role, acting both as redox mediator and as carrier of the ethylene oxidative intermediate.

Biography:

Jiaqi completed her Ph.D. in Analytical Chemistry at Iowa State University, working under the guidance of Professor Wenyu Huang. Her doctoral research was primarily centered on the design and synthesis of intermetallic nanomaterials, as well as the study of heterogeneous gas-phase thermocatalysis. Jiaqi now is a postdoctoral researcher in the Department of Chemistry and the International Institute of Nanotechnology (IIN) at Northwestern University, where she is under the mentorship of Professor Ted Sargent. In her current role, she is deeply engaged in the study of electrooxidation reactions and CO_2 electrocatalysis.

A Background Enzymatic Active Bath Affects Liquid-Liquid Phase Separation (LLPS) of Proteins

Kevin Ching

Syracuse University, Syracuse NY

Abstract Not Available!!!

Manipulation of the strong metal-support interaction (SMSI) between Pt and TiO2 by constructing TiO_2 thin layer over CeO_2-TiO_2

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[2]School of Energy and Chemical Engineering, Xiamen University Malaysia, Jalan Sunsuria, Bandar Sunsuria, Sepang, Malaysia

Abstract:

The development of highly thermal stable supported Pt based catalysts for many industrial processes, especially high temperature oxidation reactions, is still a big challenge. Herein, we report a facile strategy to prepare Pt/(TiO_2-CeO_x@TiO_2). The TiO_2 thin layer over CeO_x-TiO_2 ensured controllable strong metal-support interaction (SMSI) with Pt. It not only limited the coverage of Pt by TiO_x overlayers, but also inhibited the over oxidation of Pt species induced by the strong interaction of Pt-O-Ce. The obtained catalysts presented high stability even after 600 ^{o}C treatment in air and 600 h reaction in toluene oxidation. This work provides new insights into the effect of SMSI on supported Pt catalysts and offers a strategy to tune the Pt active phase and design highly active and thermal stable catalysts for industrial applications.

Biography:

Fu got his bachelor and PhD degree in Xiamen University. During this period, his major research is related to catalytic oxidation. In 2016-2017, Dr Fu did one-year research in the Group of Professor Graham Hutchings, Cardiff university. Before joining Xiamen University Malaysia, he worked as a postdoctoral fellow in University of Waterloo and Western University, Canada.

The End

Oral Presentation

Computational Exploration of Ammonia Synthesis on Iron

Craig Daniels1 *, Shinae Kim1 , Joy Mueller1 , Habib Najm1 , and Judit Zador1

[1]Sandia National Laboratories, USA

Abstract:

The Haber-Bosch process for ammonia synthesis is an exceedingly important catalytic process, being responsible for the production of 250 million tons of ammonia per year by some estimates. While it has been investigated extensively in both experimental and ab-initio studies, there is still some debate on which steps are rate-limiting. In addition, the complexity of the lattice and reaction processes makes defining a complete system for lattice-based Kinetic Monte Carlo (KMC) simulations challenging. We present results examining the Haber-Bosch process on BCC Fe (111) using a lattice KMC model as implemented in KinCat (https://github.com/sandialabs/kincat), a new software that is able to run KMC simulations using GPU computational resources. KinCat modeling is informed by detailed periodic DFT calculations to determine crucial transition rates. Fe(111) has 6 unique crystallographic sites adsorbed species might bind to, and it can be unclear which represents the most favorable site for a given adsorbate or reaction step. To this end, we calculate sites-specific rates using Pynta (https://github.com/zadorlab/pynta), a recent software designed to identify and calculate ratecoefficients systematically for reactions of adsorbates on metallic crystal surfaces. Pynta relies on Sella (https://github.com/zadorlab/sella), an efficient and flexible saddle point optimization software to locate transitions states. We complement our KMC results with a global sensitivity analysis of the ammonia desorption turnover frequency with respect to the process rates, identifying the most important rates to further refine to improve simulation accuracy. This work will demonstrate the power of combining recent computational tools in investigating and illuminating kinetic pathways of catalytic reactions.

Biography:

Craig Daniels earned a PhD in Materials Science and Engineering from the University of Illinois Champaign-Urbana. He is a primary developer for KinCat, an open-source 2D KMC simulator for heterogeneous catalysis. Dr. Daniels is currently a postdoc at Sandia National Laboratories (SNL) contributing to the Exascale Catalytic Chemistry Project (ecc-project.org). This project seeks to develop and apply exascale-ready computational tools to heterogeneous catalytic systems.

Scaling Up CARGEN® Technology for Multi-Walled Carbon Nanotubes and Syngas Production: An Experimental and Modeling Study

Mohamed S. Challiwala[†,€], Gasim Ibrahim[†,€,‡], Hanif A. Choudhury[†,€], Nimir O. Elbashir[€,†,*]

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‡Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, 77840, USA

Abstract:

Dry reforming of methane (DRM) offers an avenue for converting carbon dioxide (CO_2) and methane (CH_4)—the two major greenhouse gases—into syngas, a vital chemical precursor. However, DRM is constrained by high energy demands, catalyst deactivation, and an unfavorable H_2/CO ratio. Previously, a unique dual-reactor system that produces multi-walled carbon nanotubes (MWCNTs) and syngas as products was proposed. This system offers at least 65% CO_2 conversion at 50% of the energy demands of DRM. The present study experimentally proves and scales the concept from the milligram scale to the multi-gram scale and, ultimately to the multi-kilogram scale of MWCNT production. This study also introduces and experimentally validates a lumped Langmuir-Hinshelwood-Haugen-Watson (LHHW) kinetics model capturing a network of nine primary reactions involving CO, O_2, H_2, CH_4, CO_2, H_2O, and solid carbon. The model performs within a 5% error margin at the milligram scale for the carbon formation rate at 550 °C. The model is validated at 500 °C, 550 °C, and 600 °C on a multi-gram scale to capture the temperature effect. This scale's CH4-conversion and CO2-conversion predictabilities are within 8% and 30% error margins, respectively. At a multi-kilogram scale, the model predicts the carbon formation rate within a 21% error margin at 550 °C. Finally, characterization of the MWCNTs using Raman, SEM, TEM, STEM, and TGA-DTA confirms MWCNT quality consistency at all scales. in summary, it provides valuable experimental scale-up data and a kinetics model that can be a foundation for developing future commercial-scale reaction systems.

Biography:

Elbashir is a professor in the Chemical Engineering Program at Texas A&M University at Qatar and the director of Texas A&M's Gas and Fuels Research Center (GFRC). He has extensive research and teaching experience from four countries worldwide, including his previous position as a researcher at BASF R&D Catalysts. His research focuses on designing advanced reactors, catalysts, and decarbonization of gas processing plants. During the past eight years, he has established several unique global research collaboration models between academia and industry, with research funds exceeding $15m. He holds numerous patents and scientific publications. Professor Elbashir is an elected member of the Sudanese National Academy of Sciences (SNAS) and a Fellow of the American Institute of Chemical Engineering (AIChE).

Metal-Supported Solid Oxide Fuel Cell System with Infiltrated Reforming Catalyst Layer Operating under Direct Ethanol Feed Configuration

Su Ha*[1], Martinus Dewa[1, 2], Mohamed A. Elharati[1], A. Mohammed Hussain[3], Yohei Miura[4], Song Dong[4], Yosuke Fukuyama[4], Yoshihisa Furuya[3], Nilesh Dale[3], Xianghui Zhang[1], Oscar G. Marin-Flores[1], Di Wu[2], and M. Grant Norton[1,2]

[1]The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Wegner Hall Room 105, 1505, NE Stadium Way, Pullman, WA 99164

[2]School of Mechanical and Materials Engineering, Washington State University, Pullman, WA 99164, USA

[3]Nissan Technical Centre North America, Farmington Hills, MI-48335, USA

[4]Nissan Research Centre, Nissan Motor Corporation Limited, Kanagawa 237-8523, Japan

Abstract:

Metal-supported solid oxide fuel cell (MS-SOFC) has been an interest in the SOFC research in the past two decades due to its low-production cost compared to Ni-based conventional anode supported SOFC, and its mechanical robustness, especially during the rapid heat-up and cool-down. This abstract summarized the efforts done at Washington State University in collaboration with Nissan Motor Company to develop a micro-reforming catalyst layer within MS-SOFC that is capable to operate under ethanol steam reforming conditions at intermediate temperatures (600-700 °C). Without reforming catalyst, the cell would be prone to permanent deactivation caused by carbon deposit or coking due to the low catalytic activity of Ni anode towards the ethanol steam reforming reaction. Using catalyst precursor infiltration method, the both noble metal (Rh-based) and non-noble metal (NiMo-based) catalysts were applied into the MS-SOFC's porous metal structure and were greatly improved the cell operation lifetime up to 100 hours by enhancing the cell's reforming activity, maximum current density, and coke resistance, compared to the MS-SOFC without micro-reforming catalyst layer.

Biography:

Su Ha is a director and professor in the Gene and Linda Voiland School of Chemical Engineering and Bioengineering at Washington State University (WSU). He is also a director for the O.H. Reaugh Laboratory for Oil and Gas Processing Research at WSU. He joined the school in 2005 as an assistant professor after completing his Ph.D. degree in chemical engineering from the University of Illinois at Urbana-Champaign. He has published over 100 publications in the research areas of energy generation from alternative fuels. His research has been cited over 5,500 times with h-index of 30.

Catalyzing a Career in Research, Teaching, Service, and Academic Administration

Jason Keith

Mississippi State University, Mississippi State, MS

Abstract Not Available!!!!

Progress in Catalytic Cationic Polymerization

Stewart Lewis

Pyramid Polymers LLC, Zanesville, OH

Abstract Not Available!!!!

Probing Biomass-Burning-Derived Ice-Nucleating Particles Using a Microfluidic Platform for Simulating Immersion Freezing in the Atmosphere: Insights into Cloud Microphysics

Swastika S. Bithi, Sanjoy Bhattacharia, Nathan Howell, and Emily Hunt

College of Engineering, West Texas A&M University, Canyon, TX 79015.

Abstract:

Atmospheric ice-nucleating particles (INPs) serve as catalysts in cloud ice particle formation, significantly influencing cloud properties, precipitation, and climate dynamics. However, the ice nucleation process in clouds is complex and not yet fully understood. Combustion-derived minerals and soil and dust particles are essential sources of INPs in biomass-burning aerosol emissions. However, their role in the climate system is not well studied.

To bridge this knowledge gap, West Texas A&M University researchers have developed the West Texas A&M University Microfluidic Static Droplet Array (WT-MFSDA) platform. This innovative platform is specifically designed for studying ice nucleation, focusing on immersion freezing. It allows researchers to assess the ice nucleation activity of aerosols and ashes biomass combustion produces. The WT-MFSDA platform integrates a microfluidic device with interconnected droplet parking traps, a unique hand pipetting method to create an array of INP-laden nanoliter-sized droplets, and a commercial cooling unit for visualizing and characterizing freezing events of individual droplets.

Using this platform, the researchers aim to investigate the ice nucleating particles in biomass-burning bottom ash and aerosols generated from various grass, wood, and cotton waste relevant to the West Texas region. Additionally, they will use X-ray diffraction (XRD) to identify ice nucleation-active mineral phases in different ash samples. The individual particle compositions in the bioaerosol samples will be characterized using scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDX).

The comprehensive understanding of the sources and properties of INPs derived from biomass burning and insights gained through the WT-MFSDA platform will significantly improve the knowledge and modeling of INP resources, transport, and cloud microphysics. This research will have implications for both local smoke-impacted regions and the global scale, leading to a better understanding of cloud processes, precipitation patterns, and climate dynamics.

Production of Syngas from Biogas Using Electrified Steam Methane Reforming: A Pilot Plant Story

From, Thomas Norup 1+2*; Mortensen, Peter Mølgaard2 ; Partoon, Behzad1 ; Rautenbach, Marené2 ; Østberg, Martin2 ; Bentien, Anders1

[1]Department of Biological and Chemical Engineering, Aarhus University, Hangøvej 2, 8200 Aarhus N, Denmark.

[2]Topsoe A/S, 2800 Kongens Lyngby, Denmark.

Abstract:

The production of synthesis gas (syngas) for manufacturing of various bulk chemicals and fuels including hydrogen, ammonia, methanol, and liquid fuels, relies on the steam-methane-reforming (SMR) process. However, the current SMR process involves fired reformers to produce the necessary reaction heat by combustion of fossil fuels, leading to a substantial CO2 footprint. Electrification of the traditional SMR process therefore has a significant CO2 reduction potential, particularly if renewable electricity is used. This work shows first operational experience with industrial-scale electrified steam methane reforming (eSMR) technology, where biogas is used as a sustainable

carbon feedstock to produce syngas. Since the catalytic system is electrically heated in an eSMR, it eliminates the thermal restrictions inherent in the traditional SMR design. As a result, the eSMR design can achieve higher operating temperatures, greater stability, improved control and agile for dynamic changes, leading to better overall process performance. This opens new possibilities for dynamic operation, higher energy efficiency, and new configuration designs. The eSMR-biogas configuration tested in this work, providing a first-hand experience that could lead to attractive and competitive plant designs for sustainable and renewable production of chemicals and fuels.

Noncovalent Interaction-Controlled Site-selective C–H Transformations

Yoichiro Kuninobu*

Kyushu University, Japan

Abstract:

Site-selective C–H transformations are important to obtain desired compounds as single products in a highly efficient manner. However, it is generally difficult to achieve such transformations because organic substrates contain many C–H bonds with similar reactivities. Therefore, the development of practical and efficient methods for controlling site selectivity is highly desirable. The most frequently used strategy is "directing group method." Although this method is highly effective and promotes site-selective reactions, it has several limitations. Our group recently reported other methods to achieve site-selective C–H transformations using non-covalent interactions between a substrate and a reagent or a catalyst and a substrate (non-covalent method). In this lecture, I will talk about hydrogen bond- and Lewis acid-base interactioncontrolled site-selective C(sp2)–H borylation of aromatic compound. Electrostatic interactioncontrolled site-selective C(sp3)–H alkylation of anilines, amino acids and peptides will also be presented.

Biography:

He received his B.S. and Ph.D. degrees from the University of Tokyo in 1999 and 2004, respectively. He was appointed assistant professor at Okayama University in 2003. In 2012, he was promoted to an associate professor at the University of Tokyo and the group leader of ERATO project, JST. In 2017, he became a full professor at Kyushu University. His research interests relate to the creation of high-performance catalysts, the development of novel and highly efficient synthetic organic reactions, and the creation of π-conjugated molecules

Advancements in ResonantAcoustic® Continuous Flow Technology: Catalytic Applications

Joseph Mayne[1]*, Stephanie Trant[1] and Lawrence Farrar[1]

[1]Resodyn Corporation, USA

Abstract:

ResonantAcoustic® Mixing (RAM) technology is revolutionizing catalysis applications across industries like energetics, pharmaceuticals, and energy storage. This presentation highlights Resodyn's pioneering work, focusing on continuous flow synthesis powered by RAM.

RAM is a powerful non-contact mixing platform, oscillating a container and its contents at their

resonant frequency, reaching accelerations of up to 100g. Unlike mechanical mixing, RAM excels in safe mixing of a broad range materials through low-shear acoustic waves.

Resodyn's innovation has led to the RAM-based Continuous Acoustic Reactor technology. Oxygen stripping experiments show a remarkable 25% enhancement in the gas-liquid mass-transfer coefficient, while model reaction analyses reveal a 50% reduction in mixing time compared to microreactors.

Application of RAM-based mechanochemistry offers the potential to completely revolutionize the chemical industry by essentially eliminating solvent use, dramatically economizing reactant use, preventing waste, decreasing byproduct formation, and unlocking new synthetic routes.

With these advantages, Resodyn is advancing commercial deployment of automated continuous acoustic reactor and crystallizer systems, which may be tailored for catalysis applications. These turn-key systems encompass feed, product synthesis, cutting-edge Process Analytical Technologies (PATs), and product separation, adaptable to various catalytic challenges within energetics and insensitive munitions domains.

In summary, RAM technology is transforming catalysis in diverse fields by providing efficient, safe, and adaptable continuous mixing and synthesis solutions.

Biography:

Dr. Mayne, with over a decade of industrial R&D experience, received a Ph.D. in Chemical Engineering from the University of Michigan, where his thesis focused on catalysis for hydrogen generation. He also earned a B.Sc. in Chemical Engineering from the University of Utah. Dr. Mayne dedicated a decade to pioneering gas separation membranes in the natural gas industry. In his current role at Resodyn, as a Senior Chemical Engineer for 4 years, he leads the development of flow processes using ResonantAcoustic® Mixing.

Plasma assisted methane reforming

Mruthunjaya Uddi* 1 , Yue Xiao1 , Prawal Agrawal1 , Josh Kintzer1 , Chien-Hua Chen1

1Advanced Cooling Technologies, Inc., USA

Abstract:

Endothermic Dry Methane Reforming (DMR) consumes two greenhouse gases-methane and carbon dioxide-to produce syngas, a valuable product to prepare various chemicals such as liquid transportation fuels through Gas-to-Liquid (GTL) Fischer-Tropsch (FT) processes, methanol, acetyls (acetic acid), formaldehyde, formic acid, and dimethyl ether, etc. While thermal-catalytic DMR is conducted at high temperature (700–900 °C) with fossil fuel supply, Plasma assisted DMR (pDMR) can be conducted at lower temperatures (300–500 °C) using waste heat and renewable energy to produce syngas while performing carbon capture. Dielectric Barrier Discharge (DBD) plasma has been extensively investigated for its convenient scaled-up design for industrialization. However, the energy efficiency and conversion of DBD-based pDMR are still low, and considerations for potential industrial process flow integration are lacking. In recent years, we further investigated improvements in the efficiency of pDMR, including an innovative reactor design that eliminates the detrimental surface discharge and with adoption of Ni-based perovskite catalysts. The study of these various configurations, power supply, and catalysts on DMR efficiency and conversion levels will be presented from the viewpoint of plasma-catalysis synergy. We achieved a maximum conversion of methane of more than 95% and carbon dioxide conversion of 20% using plasma DMR, in a 1:9 mixture ratio of methane to carbon dioxide. The high methane conversion is designed to eliminate the separation process in a potential industrial process integration. In this case, the specific energy input of less than 11 eV/molecule was achieved. We continue to develop more efficient DMR processes.

Biography:

Uddi has over 14 years of experience in the areas of plasma catalysis, plasma-surface interaction laser diagnostics, plasma combustion, solid oxide perovskite Ion Transport Membrane chemical synthesis, and chemical looping reactions. Dr. Uddi obtained his Ph.D. in Mechanical Engineering from the Ohio State University studying plasma assisted combustion using advanced non-linear laser diagnostics.

The Wall Effect in Heterogenous Catalysis

Hubert M. Quinn

The Wrangler Group LLC, 40 Nottinghill Road, Brighton, Ma.

Abstract:

When supported catalysts are packed into conduits, there is always two opposing design criteria. On the one hand, efficient packed bed performance demands the design criterion of a large D/dp ratio. This in necessary to obtain the optimum contact between catalyst and flowing reagent stream. On the other hand, most reactions will generate heat and removal of heat demands a low D/dp value in order to optimize heat removal. However, when the D/dp ratio becomes small the so-called “wall effect” comes into play which can seriously erode the efficiency of the interactions as well as the operating pressure drop across the packed conduit. In this paper, a new fluid flow model, QFFM (Quinn Fluid Flow model), will be used to describe this wall effect phenomenon and how best to manage the tradeoff between reaction efficiency and heat control. In particular, the wall effect normalization coefficient, I, will be identified and the protocols by which its impact can be minimized. The two major contributors to the value of I, which are the viscous boundary layer and internal wall roughness, will be discussed.

Biography:

The author, Hubert M. Quinn, whose formal training is in Physics and Chemistry spent his entire career in the field of High-Pressure Liquid Chromatography (HPLC). His experteese is in the design and manufacture of packed beds containing small as well as large particles. He is responsible for development of efficient packed columns used in conjunction with Mass Spectrometry in the field of Bioanalysis of small and large molecules, of interest in the pharmaceutical industry.

A Thermodynamic Framework for the Temperature-Dependence of Enzyme-Catalyzed Biochemical Reactions

Mark Ellis Ritchie

CarbonSolve, LLC and Soils for the Future, LLC, Cicero, NY

Abstract Not Available!!!!

Upcycling PPE waste to chemical feedstocks by pyrolysis in presence of ceria based catalysts

Ross Baird[1], Raffaella Ocone[2] Aimaro Sanna[1]*

[1]School of Physical and Engineering Sciences, Heriot Watt University, Edinburgh, EH14 4AS, UK;

[2]School of Energy, Geoscience, Infrastructure and Society, Heriot Watt University, Edinburgh, EH AS, UK.

Abstract:

Single-use personal protective equipment (PPE), such as face masks and nitrile gloves, are challenging to recycle through conventional means due to the high cost of collection and processing. Due to increasing global demand for PPE, and the potential environmental impacts from these materials if processed incorrectly, there is a need to develop a sustainable and economical technology for disposal after use. Pyrolysis is currently the most common way to recover hydrocarbons from plastic and involves heating the waste to high temperature in the absence of oxygen and could be exploited for upcycling plastic into high value chemicals by tuning the resulting oil composition in the presence of catalysts and further refining. In this context, this work proposes to use coke resistant CeO_2 doped with yttria and gadolinium for the pyrolysis of PPE plastic waste in a fixed bed at 700 °C and ambient pressure. The results indicate that the ceria-based catalysts increase cracking to CO and C_2/C_3 hydrocarbons and enhance the recovery of cycloalkanes and esters while lowering the content of ketones and amines compared to the uncatalyzed run. Both catalysts were seen to significantly increase the wax and diesel range fractions in the oil from 50% (without catalyst) to 80% at the expense of gasoline with the Gd doped catalyst resulting in about 17% cyclohexanes. Therefore, Gd/CeO_2 could be used to expand the applications of PPE waste derived bio-oil.

Biography:

Since 2018 Dr Aimaro Sanna is an Assistant Professor at the Institute of Mechanical, Process and Energy Engineering (IMPEE), Heriot-Watt University (HWU). He did his PhD in Chemical and Environmental Engineering at the University of Nottingham working on catalytic pyrolysis and bio-oil hydrotreating. He worked as post-doctoral researcher at the University of Nottingham and HWU on clean fuels technologies and then, he was awarded the Heriot-Watt Research Fellowship (2014-2017). His research team is developing novel catalytic systems to produce hydrogen, renewable liquid fuels and commodity chemicals out of lignocellulosic and plastic wastes.

Leveraging The Aqueous Chemistry of Fe for Pharmaceutical Design

Eric M. Gale

Martinos Center for Biomedical Imaging, Massachusetts General Hospital and Harvard Medical School, USA

Abstract:

In aqueous solution, iron (Fe) can adopt different oxidation states and engage in diverse chemical speciation with discrete complexes exhibiting distinct magnetic properties. We are capitalizing on this rich chemistry to develop magnetic resonance (MR) imaging probes to noninvasively detect, map, and quantify pathologic processes occurring at cell and molecular level. This talk will focus on chemistry we have developed toward this objective. I will discuss ligand design that enables precision control and stimuli-driven switching between μ-oxo bridged antiferromagnetically coupled and mononuclear high-spin paramagnetic complexes of Fe(III). I will also discuss new chemistry to simultaneously stabilize and enable switching between MR silent Fe(II) and strongly MR visible high-spin Fe(III) complexes, which require disparate and distinct ligand-donor environments.

Biography:

Eric Gale received his PhD in chemistry in 2012 from the University of Georgia under the mentorship of Dr. Todd Harrop. Eric pursued postdoctoral training between 2012-2015 at Massachusetts General Hospital/ Harvard Medical School under the mentorship of Dr. Peter Caravan, where he learned to leverage his chemistry background in inorganic chemistry towards pharmaceutical development. He is currently an Assistant Professor in Radiology at MGH/ HMS, where he has established an externally funded research group that applies chemistry to solve unmet challenges in biotechnology.

The PIPK lipid kinase family: catalytic mechanism and inhibition

Ya Ha[1]*, Song Chen[1], Caroline Chandra Tjin[2], Yagmur Muftuoglu[1], Zunyu He[1], Jonathan Ellman[2]

[1]Yale School of Medicine, USA; [2]Yale University, USA

Abstract:

The phosphatidylinositol phosphate kinase (PIPK) family of enzymes converts singly phosphorylated phosphoinositides to phosphatidylinositol bisphosphates PI(4,5)P_2 and PI(3,5)P_2. The type 1, 2 and 3 PIPKs are highly similar in their kinase domains but differ in catalytic activity and biological function. We have identified a structural motif unique to the PIPK family that serves to recognize the monophosphate on the lipid substrate. The exquisite catalytic specificity among family members is determined by the common, but subtly different, monophosphate binding site and a divergent specificity loop, the latter of which recognizes different orientations of the lipid's inositol head group. The PIPKs have evolved structural features different from protein kinases that allow catalysis at close proximity to the membrane surface, and some of these features were exploited to develop highly selective chemical probes. The PIPK inhibitors are potentially useful in treating metabolic disorders, cancer and viral diseases (e.g., COVID-19).

Biography:

B.S. Biochemistry, Nanjing University, China, 1992

Ph.D. Biochemistry & Biophysics, University of Minnesota Twin Cities, USA, 1998

Protein Energy Landscapes and Enzyme Catalysis – Dynamic Control of the Active Site via Distal Mutations

Joerg Zimmermann

Loyola University Chicago, Chicago, IL

Abstract Not Available!!!!

BioManufacturing 2.0: Cell Free Enzymatic Synthesis of Commodity and Specialty Chemicals

Paul Opgenorth

Invizyne Technologies Inc. (Monrovia, California)

Abstract:

Over the last decade, Invizyne's has pioneered technology that assembles entire biosynthetic pathways cell free, that turn cheap substrates to products using previously isolated enzymes and represents a paradigm shift for the bio-based production of chemicals. In this fashion, we effectively separate the traditional one stage fermentation-based process into two stages, 1) the catalyst (enzyme) production; and 2) the cell free reaction. Breaking down this problem into two stages allows us to optimize each stage individually and drive efficiencies from both the enzyme production and the cell free reaction without having to deal with cell toxicity / viability issues.

Invizye has implemented the cell-free approach to produce terpenes, isobutanol, bioplastic, and prenylated natural products with production parameters that exceed what has been possible in cells. Indeed, members of Invizyne have recently achieved production metrics that already surpass even highly evolved ethanol production in yeast. In particular, Invizyne can now produce the next generation biofuel, isobutanol, cell free at 275 g/L over 100 hours at a maximum productivity of 4 g/L/h with a yield of >90% of theoretical. This talk will highlight the milestones towards developing cell free enzymatic synthesis for commodity and specialty chemicals.

Biography:

Dr. Opgenorth has served as Director of Research and Development of the Company since August 2019. From May 2017 to August 2019 Dr. Opgenorth was a postdoctoral scientist in the Joint BioEnergy Institute at Lawrence Berkeley National Lab. Dr. Opgenorth received his PhD in Chemistry, Biochemistry, and Structural Biology from the University of California, Los Angeles in 2015, and Bachelor of Science in 2004 in Chemistry from the University of California, Davis

Engineered Biocatalysis in the Era of Synthetic Biology and AI

A. Joe Shaw

Manus Bio, Waltham, MA

Abstract Not Available!!!!

Molecular Glues vs PROTAC Drugs, Future of Targeted Protein Degradation Therapy

Tauseef Butt

Progenra Inc, Malvern, PA

Abstract Not Available!!!!

Directed evolution of laccase by protein display with *Bacillus subtilis* spores.

Edgardo T. Farinas*

New Jersey Institute Technology, Department of Chemistry and Environmental Science, USA United States

Abstract:

Bacillus subtilis spores offer several advantages that make them attractive for protein display. For example, protein folding issues associated with unfolded polypeptide chains crossing membranes are circumvented. In addition, they can withstand physical and chemical extremes such as heat, desiccation, radiation, ultraviolet light, and oxidizing agents. As a result, the sequence of the displayed protein can be easily obtained even under harsh screening conditions. Next, immobilized proteins have many economic and technological advantages. They can be easily separated from the reaction and the protein stability is increased in harsh environments. In addition, they can be easily separated from the reaction, and the protein stability is increased in harsh environments. Spores are also amenable to high-throughput screening for protein engineering and optimization. *B. subtilis* coat protein CotC is a laccase and it catalyzes oxidation reactions in a wide range of substrates, which is coupled to four-electron reduction of O_2 to H_2O. Directed evolution was used to construct CotA libraries and expressed on the spore coat. Libraries were assayed for substrate specificity, organic solvent stability, and pH stability. In all cases, improved variants were isolated. In conclusion. Spore displayed proteins can be used in a wide array of biotechnological and industrial applications such as vaccines, bioabsorbants to remove toxic chemicals, whole-cell catalysts, bioremediation, and biosensors. Lastly, spores are easily produced in large quantities, have a good safety record, and can be used as additives in foods and drugs.

Biography:

Edgardo Farinas is an Associate Professor at the New Jersey Institute of Technology. He received a Ph.D. from the University of California at Santa Cruz (inorganic chemistry). This was followed with postdoctoral research at Yale University (rational protein design), California Institute of Technology (directed evolution), and University of Texas at Austin (*Escherichia coli* protein display). His current interests include protein engineering and optimization and machine learning.

Production of lipase activity biocatalyst by enzyme immobilization on a graphite-residual inert support

Mariana Valdez-Castillo[1,2]*, Dominique Oumattu[1], Beatriz Delgado Cano[1], Michèle Heitz[2], Antonio Avalos Ramirez[1]

[1]Centre National en Électrochimie et en Technologies Environnementales, Canada.

[2]Département de génie chimique et de génie biotechnologique-Université de Sherbrooke, Canada.

Abstract:

Detergents are complex formulations containing petroleum-derived hydrocarbons as emulsifiers, solvents, and surfactants, being the latest the key components of cleaning product formulations. However, surfactants derived from petroleum hydrocarbons represent a potential environmental risk because they act as chelating agents of heavy metals, increasing their recalcitrant and toxic effects on ecosystems and human health. Surfactants can also cause disruption of lipid cells membrane, leading to the development of skin, eyes, and respiratory system diseases.

Currently, the use of enzymes as replacements of petroleum-derived surfactants (PDS) is a promising research area. Among these enzymes, lipases can hydrolyze carboxylic ester bonds of lipids and catalyze reactions of esterification, interesterification, and transesterification, which increases the interest of the detergent industry to use them as biodegradable alternative to the PDS. The lipase activity is a pivotal parameter for the formulation of detergents. Lipase activity can be improved by means of lipase immobilization, which increases the contact surface area between lipids and lipase. This study aimed to develop new biocatalysts by means of passive immobilization of lipase enzymes on graphite-residual particles as support. The support was functionalized with glutaraldehyde to increase lipase bonding on graphite surface. Preliminary results show the increase of enzymatic activity up to 476 U/mg, which was twice higher than non-immobilized lipase. This represents new ways of valorization for residues from recycling processes, contributing to the concept of circular economy.

Biography:

Mariana Valdez-Castillo is postdoctoral researcher focused on the development of bioprocesses for the valorization of agro-industrial residues into biocombustibles and biomolecules of industrial interest. She also has experience with the synthesis and characterization of nanomaterials to treat air contaminants, such as bioaerosols, by photocatalytic methods. She holds a Ph.D. in water sciences issued by the Institute national de la recherche scientifique (Canada, 2022). She also holds a master's degree in environmental sciences focused on biotechnology and engineering issued from the IPICYT (Mexico, 2018). Graduated with honors from the IPN in environmental engineering (Mexico, 2015).

Development of CSM Recovery Methods Based on their Adsorption on Biocomposites Containing Peptides

Beatriz Delgado Cano

CNETE, Canada

Abstract Not Available!!!!

Obtaining Catalyst Design Rules for CO2 Hydrogenation via Machine Learning Tools

Mohammad Khatamirad1*, Edvin Fako2 , Sandip De2 , Chiara Boscagli3 , Matthias Müller3 , Fabian Ebert1 , Raoul Naumann d'Alnoncourt1 , Ansgar Schaefer2 , Stephan Andreas Schunk2,3,4, Ivana Jevtovikj3 , Frank Rosowski1,2

[1]BasCat – UniCat BASF JointLab, Germany;

[2]BASF SE, Group Research, Germany;

[3]hte GmbH, Germany;

[4]Institute of Chemical Technology, Universität Leipzig, Germany)

Abstract:

In recent years, In-based catalysts have gained popularity for their promising performance in catalytic conversion of CO2 to methanol, while showing higherstability under CO2-rich conditions, compared to the benchmarked Cu-based catalysts. However, obtaining high selectivity for desired products such as methanol and DME requires further improvement of this system. Conventional catalyst design is bottlenecked by circular dependency between synthesis, test and characterization. To address these challenges, in our study we set out to obtain catalyst design rules which facilitate accelerated material discovery and reduce resource-dependency of the design process. We prepared 13 In-modified catalysts via incorporation of promoter elements onto the reference In/ZrO2, and tested each catalyst for CO2 hydrogenation to methanol. In parallel, with help of unsupervised machine learning (ML) methods, major reaction intermediates along two hypothesized competing reaction pathways were sampled for each catalyst. The adsorption energy of each intermediate was then computed via a DFT model. We applied the SISSO (Sure Independence and Sparsifying Operator) algorithm to increase the feature space by considering non-linear combinations of DFT-computed descriptors. These data were then combined with experimental data to construct a model for predicting catalytic performance, through detecting the most significant features. By applying the AI approach Subgroup Discovery, we then defined quantitative constraints on the values of model features, which define unique behavior. In our talk, we discuss how this combined ML and experimental approach aids accelerated catalyst design, while reducing computational cost.

Biography:

Mohammad Khatamirad obtained his B.Sc. in Chemical Engineering from Sharif University of Technology in Tehran, and his M.Sc. in Advanced Materials from Ulm University in Germany. He started his PhD at Technical University of Berlin in September 2019, with focus on data-driven catalyst design. His work as a PhD candidate has resulted in four publications, about syngas to ethanol and CO2 to methanol reactions. His PhD defense date is estimated for October 2023.

The End

Oral Presentation

Rational Design of Single-Atom Electrocatalysts for CO_2 Recycling via Quantum Mechanical Simulations

Qing Zhao* and Colin Gallagher

Northeastern University, Chemical Engineering Department, USA

Abstract:

Electrochemical carbon dioxide reduction (CO_2R) could contribute to a circular economy that will curtail unsustainable fossil fuel burning and decrease future greenhouse gas emissions. However, practical electrocatalysts for this reaction still do not exist. Single-atom catalysts (SACs) embedded in doped graphene are emergent catalytic materials that unite the scalability of heterogeneous catalysts with the activity, selectivity, and atom-economy of homogeneous catalysts, yet their applications in catalyzing CO_2 conversion remain unclear. In this work, we study the effects of active transition metal centers and dopants of SACs on tuning reactivity of electrochemical CO_2 reduction using quantum mechanical simulations, namely density functional theory. As a result of the modified electronic properties via varying metal-coordination environment, we identified several SACs as active and selective electrocatalysts for CO_2 conversion. In addition, we develop new design principles of introducing heteoatom doping and dual-metal site in SACs to further improve their catalytic performance. Our work sheds light on ways to enhance SACs activity via multiple strategies towards discovering practical electrocatalysts for CO_2 conversion to achieve a carbon-neutral economy.

Fuel Reforming and Desulfurizing Needs for Solid Oxide Fuel Cells

Yanhai Du

Kent State University, Kent, OH

Abstract Not Available!!!!

Design Considerations for Catalysis Relevant to Energy Storage

Amy C. Marschilok,[1,2]* Esther S. Takeuchi, [1,2] Kenneth J. Takeuchi[1,2]

[1]Stony Brook University, Stony Brook, NY, 11794, USA

[2]Brookhaven National Laboratory, Upton, NY, 11973, USA

Abstract:

Metal air batteries fall into a special category as the electroactive cathode material, oxygen (O_2), is available in excess from outside the battery where it does not contribute to the initial mass or volume of the battery. Thus, metal air batteries have very high energy

density compared to fully sealed battery systems. For a reversible system, catalysts provide benefit to reduce the overpotential of both the oxygen reduction reaction (ORR) as well as the oxygen evolution reaction (OER). Further, the structure of the air electrode can be varied to address kinetic issues. The three-phase electrode-electrolyte-oxygen interface is critical a determinant of the activity, where each component plays an

important role. The nature of the catalyst is important as well as the local and mesoscale environment to enable appropriate functionality. The catalysts as well as the structures supporting the catalysis will be discussed considering dimensionality where two-dimensional as well as three-dimensional constructs and the associated functionality will be described. This talk focuses on an important aspect of electrocatalysis considering the nature of the material as well as how the surroundings influence behavior.

Biography:

Amy Marschilok is a Professor of Chemistry at Stony Brook University and holds a joint appointment as Energy Storage and Systems Division Manager at Brookhaven National Laboratory. She is the Director of the Center for Mesoscale Transport Properties, a DOE funded Energy Frontier Research Center. She was in the inaugural cohort of the DOE Oppenheimer Science and Energy Leadership Program, was honored by the DOE Energy Storage Grand Challenge Celebration of Women's History Month, is on the Board of Directors of the Society of Electroanalytical Chemistry, and was inducted into the National Academy of Inventors Stony Brook University Chapter.

Next Generation Batteries: Impacts on Materials Needs

Kenneth J Takeuchi,[1,2]* Amy C. Marschilok,[1,2] Esther S. Takeuchi[1,2]

[1]Stony Brook University, Stony Brook, NY, USA

[2]Brookhaven National Laboratory, Upton, NY, USA

Abstract:

Currently, lithium ion batteries dominate the market where they are extensively used for portable electronics and the growing application for electric vehicles. The lithium-ion battery, the subject of the 2019 Nobel Prize in Chemistry, was a remarkable advance where its battery behavior has been described as rocking chair or topotactic, as lithium ions shuttle between the positive and negative electrode and the crystallographic structures at the positive and negative electrode are largely maintained. However, an emerging application for batteries for large scale low cost storage intended for integration with renewable energy generation such as wind and solar demands consideration of alternatives. The inherent intermittency of renewable energy requires the use of storage where battery alternatives based on low cost earth abundant sustainable materials that are also less flammable than current lithium ion systems would be beneficial. This presentation will highlight progress towards safe, environmentally sustainable non-topotactic batteries based on manganese oxide where the findings have implications for the manufacture of the materials and components needed for these types of batteries.

Biography:

Kenneth J. Takeuchi is a SUNY Distinguished Teaching Professor at Stony Brook University with a joint appointment at Brookhaven National Laboratory. His extensive expertise encompasses inorganic coordination chemistry, materials science and understanding structure-function relationships. He is a Fellow of the American Association for the Advancement of Science and the American Chemical Society. He is recipient of the Responsible Care National Catalyst Award from the Chemical Manufacturers Association, the New York State recipient of U.S. Professor of the Year Award from the Carnegie Foundation, and National runner up for the Inspire Integrity Award from the National Society of Collegiate Scholars.

X-ray Spectroscopy for Advanced Investigation of Energy Materials

Chung-Li Dong

Tamkang University, Taiwan

Abstract Not Available!!!!

A Polarization Consistent Framework to Describe Photoinduced Charge and Energy Transfer Processes

Barry Dunietz

Kent State University, Kent, OH

Abstract Not Available!!!!

Tuning Catalysts for Green Design and Applications

Emily A. A. Jarvis* and Kristal Stevens[1]

Department of Chemistry and Biochemistry, Loyola Marymount University, USA

[1]Scripps Research, USA

Abstract:

Catalysts are essential in allowing greener syntheses and reactions across nearly every aspect of chemistry. Unfortunately, catalysts themselves often include rare metals and non-ideal ligands frustrating truly green design. We use density functional calculations to explore a series of ruthenium mononuclear water oxidation photocatalysts alongside an analogous series of proposed iron catalysts to investigate the feasibility of replacing costly and rare ruthenium with an earth-abundant similar metal. With strategic choice of ligands, we see promising energetic similarities between iron and ruthenium across the most challenging steps of a common water oxidation mechanism. For robust and inexpensive catalysis at scale, heterogeneous catalysis via metal oxide nanopowders is even more appealing. We discuss experimental and computational analysis of metal oxide nanopowders showing non-stoichiometric surface chemistry that would be thermodynamically unfavorable for macroscopic surfaces and consider implications for tuning the surface structure for nanopowder catalyst design.

Biography :

Emily Jarvis is a Professor of Chemistry and Biochemistry at Loyola Marymount University. Prior to joining LMU, she was a professor at Gordon College and was a National Research Council Postdoctoral Fellow at the National Institute of Standards and Technology and served as an American Chemical Society/American Association for the Advancement of Science Congressional Policy Fellow in the U. S. Senate. Her research interests include first principles computational chemistry, machine learning and green chemistry as well as science policy and sustainability. In addition to physical chemistry topics, she teaches special topics in wine chemistry and entrepreneurship and sustainable innovation.

Evaluation of reaction conditions to enhance the lactic acid yield in the hydroxyacetone oxidation over the Cu/ZrO_2 catalyst

Julio Colmenares-Zerpa[1,2], Giancarlo Gonzalez[1], A.F. Peixoto[3], Monize Picinini[4], E.A. Urquieta-Gonzalez[4], J.B.O. Santos[4], R.J. Chimentão[1*]

[1]Universidad de Concepción, Chile;

[2]Universidad de Los Andes, Venezuela;

[3]Universidade do Porto, Portugal;

[4]Universide Federal de São Carlos, Brasil

Abstract:

Lactic acid (LA) is a very important platform molecule in the chemical industry. The oxidation of hydroxyacetone (HA) to LA emerges as an environmentally friendly chemical route. This research explores the HA oxidation on the Cu/ZrO_2 catalyst searching for reaction conditions to increase the LA yield. The 5% Cu/ZrO_2 catalyst was prepared by incipient impregnation. The material was characterized by N_2-physisorption, XRD, N_2O chemisorption, NH_3-TPD, Pyridine FTIR, XPS, and H_2-TPR. Prior to the catalytic tests the solid was reduced in H_2 flow in a fixed bed quartz reactor up to 400 °C for 4 h. Different reaction conditions were tested: (i) Temperatures (90, 105, 120 and 150 °C), (ii) Concentrations of HA aqueous solution (0.5, 2, 5, 7 and 10% wt.), and (iii) Masses of HA aqueous solution (60, 120 and 150 g). The reactions were carried out in a Parr 4760 reactor with 5% O_2/N_2. N_2-physisorption showed a slight drop in the textural parameters of the Cu/ZrO_2 compared to ZrO_2. XRD of the Cu/ZrO_2 showed only characteristic peaks of the ZrO_2 tetragonal phase with no evidence of any other additional phase formed. The copper catalyst acidity measured by NH_3-TPD was 236 $\mu molg^{-1}$ whereas Pyridine FTIR quantified a Lewis acidity of 134 $\mu mol \cdot g^{-1}$. The temperature of 120 °C showed the best compromise in terms of LA yield. At this reaction temperature, the yield towards LA was visibly favored with 0.5% wt. of an HA aqueous solution. Finally, the lowest mass of HA solution (60 g) favored the yield towards LA.

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 at the Laboratory for Chemical Technology at the Ghent University (Belgium). He was an Assistant

Professor at the Faculty of Chemical Sciences of Universidad de Concepcion (Chile) from 2016 to 2022 and at present he has become an Associate professor.

A Step Towards Process Electrification: Microwave-assisted Co-Gasification of Waste Plastics and Biomass to Produce Clean Energy

Ashraf Abedin

NETL, U.S. Department of Energy, Morgantown, WV

Abstract Not Available!!!!

Fast and reliable methods of calculation of solvation energies

Sergei F. Vyboishchikov*

Institut de Química Computacional i Catàlisi and Departament de Química, Universitat de Girona, Spain

Abstract:

We proposed a family of efficient and accurate methods for calculating *solvation free energy* ΔG°_{solv} of molecules and ions both in aqueous and non-aqueous solutions. The principal version of the method (uESE – *universal Easy Solvation Evaluation*)[1–3] requires gas-phase atomic charges only. The COSMO[4] electrostatic energy E_{elst} is supplemented by correction terms (cavitation energy, van der Waals and specific interactions).

Employing DFT-derived charges,[5,6] uESE exhibits an excellent accuracy at a low computational cost. A further increase of efficiency is achieved with semiempirical charges.[7,8] However, the accuracy is then partly sacrificed.

A rapid yet accurate scheme for ΔG°_{solv} calculation can be based on a Dense Neural Network (ESE-EE-DNN) using E_{elst}, cavity surfaces, surface charges, and solvent characteristics.[10]

A number of practical applications to catalytic reaction mechanisms will be shown.

References:

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[10] Vyboishchikov, *J. Chem. Inf. Model.*, **2023**, *63*, *in press*.

Biography:

Sergei Vyboishchikov received his Diploma (=MSc) in Chemistry from Moscow State University, Russia, and his PhD in Theoretical Chemistry from the University of Marburg, Germany. In 2004 he joined the faculty of the University of Girona, Spain, where he is currently an associate professor. Dr. Vyboishchikov's research interests lie in development of density-functional and energy decomposition methods, charge schemes, and, more recently, in solvation energy methods, as well as in studies of chemical reaction mechanisms.

Steering biomass waste to value-added biofuels under facile condition by hydrochar-based nanocatalysts

[1,2] Chao Gai* , [2] Keiichi Tomishige, [1] Zhengang Liu

[1] Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, China

[2] Department of Applied Chemistry, School of Engineering, Tohoku University, Japan

Abstract:

Of the versatile strategies that satisfy the world's appetite for energy, prevent disruptive depletion of natural mineral assets, as well as minimize and remediate emissions, exploration of selected biofuels or platform chemicals from abundant, inexpensive and renewable biomass waste is one of the most environmentally responsible and economically viable option. As such, the significant promise of hydrogen as an alternative energy carrier has led to the question of how to produce hydrogen more efficiently and sustainably. This question has arisen in parallel with the development of innovative, sustainable nanomaterials that achieve desirable performance in this area with limited environmental impact. Conventional synthetic protocol for the supported metal catalysts generally require reductants (like H_2 or NaBH) and organic additives (e.g., sulphur- or nitrogen-containing organic compounds) for stabilizing metal species to prevent metal aggregation/ coke deposition. Here, we demonstrate a facile and general methodology for the one-pot fabrication of hydrochar-supported, metal nanocatalysts derived from lignocellulosic matrix with tailored composition, size and shape. Benefiting from the redox-active property of the hydrochar support, that is, promoting the in-situ reduction of metal ions during the one-step hydrothermal processing, the catalysts exhibit extraordinary catalytic activity towards efficient hydrogen-rich syngas production and tar reduction from the gasification of multiple biomass waste (e.g. sewage sludge) under mild conditions. Moreover, this strategy works without the use of any reductants/ organic additives and leads to metal nanoparticles in a uniform dispersion with promising sinter-resistant ability given that the strengthened meta-support interactions.

Biography:

Dr. Chao Gai is an Associate Professor at the Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences (RCEES, CAS). He received his Ph.D. degree from Shandong University in 2014. Then he was appointed as an Assistant Professor at the RCEES, CAS and became an Associate Professor since 2021. Now he is working at Tohoku University as a JSPS Overseas Research Fellow. He has co-authored over 60 peer reviewed papers, 2 book chapters and 20 Chinese patents (Citation over 2000; h-index 31).

Numerical Simulation of Complex Fluid Flows using Neural Networks

Jianying Zhang

Western Washington University, USA

Abstract:

Bingham fluids are a class of non-Newtonian fluids with yield stresses. They possess both solid and liquid phases separated by implicitly defined non-physical yield surfaces. Due to the unknown shapes and locations of yield surfaces, the viscous terms in the corresponding governing equations cannot be explicitly expressed, which makes the standard numerical discretization challenging. The variational reformulation established in the pioneer work of Duvaut and Lions, coupled with an augmented Lagrange method (ALM), brought about a finite element method for the flow simulation. However, local mesh refinement and preconditioning of the resulting large-scaled ill-conditioned linear system can be involved. Physics-informed neural networks (PINNs) have emerged as scientific deep learning techniques in numerical PDEs. The meshfree feature of PINNs is potentially advantageous when it comes to computation over complex geometries and solving free boundary problems. In this talk, I will present a newly developed ALM-PINN approach that incorporates the ALM into a PINN to alleviate the mesh-induced issues in the regular ALM. Numerical results will follow to validate the proposed scheme.

Biography:

Ph.D. in applied mathematics from University of California, Santa Barbara.

PIAM Postdoctoral Fellow in applied mathematics at University of British Columbia.

Currently an associate professor in Department of Mathematics at Western Washington University.

Research interests: Numerical methods for complex fluid flow and reaction diffusion models, Physics-informed neural networks.

Green Catalysis Examples and Insights from the Caribbean

Michael Forde

The University of The West Indies, Trinidad and Tobago

Abstract Not Available!!!!

Theoretical study on CH_4 activation and conversion by different catalysts

Hou-Jen Lai, Santhanamoorthi Nachimuthu, Guan-Cheng Xie, and Jyh-Chiang Jiang*

Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan

Abstract:

Despite significant progress in low-temperature methane activation, commercial viability, specifically obtaining high yields of C1/C2 products, remains a challenge. High desorption energy (>2 eV) and overoxidation of the target products are fundamental limitations in CH_4 utilization.

Herein, Herein, we report a 2 wt % Ir/TiO_2 catalyst that exhibits high methane conversion activity in low-temperature SRM with a relatively high turnover frequency (TOF) and a low activation energy compared to the literature. Long-term catalyst stability tests demonstrate an excellent resistance to coking and sintering during low-temperature SRM reactions. Furthermore, we employ first-principles density functional theory (DFT) and microkinetics simulations to investigate the CH_4 activation and the feasibility of its conversion to C_2H_4 on the RuO_2 (110) surface. In addition, the kinetics of the complete MTM (methane to methanol) oxidation cycle over Cu_2O_2/MIL-53(Al) have been studied using both DFT and microkinetic simulation methods.

Biography:

Jyh-Chiang Jiang graduated from National Taiwan University in 1986 with a B.S. in Chemistry and received his Ph.D. in Chemistry in 1994. After working as a postdoctoral fellow at IAMS, Dr. Jiang joined the faculty of the National Taiwan University of Science and Technology (NTUST) in 2001. He focuses on the theoretical and computational chemistry study of heterogeneous catalysis, optoelectronic materials, and Li-ion batteries. He has more than 220 papers in peer-reviewed journals. His research has also resulted in 4 patents. Dr. Jiang has been chairman of the Taiwan Theoretical and Computational Molecular Sciences Association from August 2019 to July 2023.

Synthesis of FAU Zeolite to Capture CO_2

Shaneela Nosheen[1]*, and Daniela M. Morales Acosta[2]

[1]Department of Chemistry and Biochemistry/ Southern Connecticut State University;

[2]Institute of Material Science/ University of Connecticut.

Abstract:

To capture CO_2 using hydrothermally synthesized highly crystalline, nanosized, and unique morphologies-based Faujasite (FAU) zeolites, we report the synthesis of single-phase highly crystalline nano-sized FAU zeolite in 3 hours. The synthesis of FAU zeolite was achieved by using a novel method of mixing two initial solutions i.e., silicates and aluminates using nano mist sprayers. Both silicate and aluminate solutions were mixed simultaneously as an aerosol or a mist. The silicate and aluminate solution mists were collected and stirred for seven days at room temperature for the nucleation process. Proper mixing resulted in suspensions of nanometer-sized gel particles. We studied the effect of synthesis time and temperature on the crystallinity of FAU. The synthesis temperature was set at 100 ^{0}C and the time of synthesis was varied from 3 hours to 6 hours. Novel nano mist solutions significantly accelerated the crystallization and eliminated the formation of impurity phases. The pure Fau phase was synthesized only in 3 hours. We noticed the presence of other phases on the X-Ray profiles when we synthesized another batch but instead of nano mist spray mixing, we added all solutions together. The SEM micrographs showed the synthesis of nanosized crystallites of Fau zeolites.

Biography:

Dr. Nosheen received her Ph.D. from the University of Connecticut in inorganic chemistry. Her research interests are the synthesis and application of nanomaterials like zeolite, titanates, and metal oxides. She joined Southern Connecticut State University in 2022 as an Assistant Professor in the Chemistry and Biochemistry Department.

Catalytic Depolymerization of Lignin into Aviation Fuel Range Chemicals Guided by Inverse Molecular Design Theory

Dequan Xiao

Center for Integrative Materials Discovery, Department of Chemistry and Chemical Engineering, University of New Haven, West Haven, CT

Abstract:

Designing sustainable heterogenous catalysts is the key for converting lignin biomass into liquid fuels. However, catalyst design remains a grand challenge in computation or experiment, due to the vast numbers of possible variables (e.g., chemical compositions and particle size of catalytic domains) in the chemical space of catalytic structure. In this work, we demonstrate an effective integrative approach of heterogenous catalyst design, guided by the inverse molecular design theory in the framework of tight-binding electronic structure theory [J. Phys. Chem. 123(46), **2019**, 10019]. The inverse molecular design (IMD) theory aims at searching for optimum catalytic properties using deterministic optimization techniques along the hypersurface of catalysis-structure, and then mapping out the catalytic structures at the optimum points, leading to a very efficient way to accelerate catalyst design. By this approach, we successfully designed a novel CuFeZn nanoalloy catalyst for converting lignin into small-molecule aromatics. By catalyst characterizations and reaction analysis in experiments, the designed nanoalloy was verified to be significantly more active than the reference Cu nanocatalyst. Due to its high activity of hydrogenation at low temperature, value-added chemicals with multiple functional groups (e.g., polymer building blocks) were obtained. Our results indicated that the inverse molecular design approach is a promising artificial intelligent solution to accelerate the search of optimum catalysts for converting lignin (a sustainable chemical resource) to value-added chemicals. In addition, the sought trimetallic catalytic systems (CuFeM) has shown to be effective hydrogenation catalysts for simultaneous conversions of CO_2 and PET polymer wastes [Angewandte Chemie 134 (10), **2022**, e202117205].

Biography:

Dequan Xiao earned his PhD in theoretical and computational chemistry at Duke University in 2009, with a BS in chemistry from Sichuan University (China) in 1996. He completed a postdoc training at Yale University from 2009 to 2013. He joined the University of New Haven as an assistant professor in 2019, he is now the endowed Buckman Chair associate professor (tenured). He serves as the department Chair. He published 119 research articles and reviews, with 5,722 citations (Google Scholar). His research was funded by NSF, USDA, DOE, CT State, and industry partners. He is interested in developing and integrating theoretical and computational chemistry methods with experiments to discover catalysts, polymer materials, and molecular drugs. He developed AI-driven catalyst design based on inverse molecular design theory, vibration-coupled electron transfer kinetics theory, and data-driven design of polymer complexes.

NON-OXIDATIVE DEHYDROAROMATIZATION OF LINEAR-CHAIN ALKANES ON INTERMETALLIC SURFACE

Ranjan Kumar Behera[1], Wenyu Huang[1,2]

[1]Department of Chemistry, Iowa State University, Ames, IA, USA

[2]US DOE, Ames Laboratory, Iowa State University, Ames, IA, USA

Abstract:

Dehydrogenation technologies have gained significant attention industrially to produce fine chemicals. Under non-oxidative reaction conditions, these processes are typically endothermic and thus require high temperature (>600 °C). Besides, low product selectivity due to various side reactions (isomerization, cracking etc.) pose significant challenges in developing novel catalytic systems. Herein, we have demonstrated Pt-based intermetallic nanoparticles (iNPs) as a highly active and, more importantly, selective catalyst for non-oxidative dehydroaromatization of long-chain alkanes to aromatized products of benzene-toluene-xylenes (BTX) family. At a reaction temperature of 550 °C, Pt based intermetallic catalysts have shown superior activity and selectivity compared to monometallic Pt nanoparticles (NPs). For the dehydroaromatization of C6-C8 linear chain alkanes, the intermetallic catalysts yield BTX selectivity of 88, 92, and 93%, respectively. Kinetics of dehydroaromatization reaction for n-hexane, including activation energy calculations, have shown that the reaction barrier is much lower on the intermetallic surface (~ 88 kJ/mol) than the monometallic Pt surface. First-order dehydroaromatization kinetics models have demonstrated that the deactivation constant on Pt surface is one order of magnitude higher than that of the intermetallic catalysts. Furthermore, using a combination of in-situ MS analysis and rate order calculations for the dehydroaromatization of various reaction intermediates, we have developed a mechanistic understanding of the dehydroaromatization process on Pt based iNPs. These results were further supported by in-situ DRIFTS studies on Pt based intermetallics. Overall, these results have provided a platform for developing novel bimetallic catalysts for efficient and selective dehydroaromatization processes as well as provided mechanistic insights into the dehydroaromatization process of linear alkanes.

Green H2 derived electricity from reacting water and aluminum catalyzed by sodium hydroxide

José V. C. Vargas1* , Henrique P. Guerra1 , Rodrigo C. Raimundo1 , Dhyogo M. Taher1 , Lauber S. Martins2 , Stephan H. Och1 , Diogo B. Pitz1 , André B. Mariano1 , Lucio Cardozo-Filho3 , Juan C. Ordonez4

1Federal University of Parana, Brazil;

2Advent Health University, USA;

3Maringa State University, Brazil;

4Florida State University, USA

Abstract:

This study introduces a mathematical model of a sustainable energy generation system comprised of a hydrogen (H2) generation reactor using recyclable aluminum and water. The system is composed of a batch reactor for greenhouse gas-free hydrogen generation, a gas-liquid separator, a buffer tank, an air booster compressor, a low-pressure filter, a hydrogen storage tank, and a 5 kW proton exchange membrane fuel cell (PEMFC) stack. A transient mathematical model for hydrogen and electricity generation was conceived based on mass and energy conservation principles, and experimentally validated. A mobile system prototype mounted on an automotive trailer was developed for granting extended range to electric vehicles or even total independence

of battery charging stations, provided that aluminum, water and catalyst (NaOH) are available. The analysis revealed that there is an optimum catalytic aqueous solution (NaOH(aq)) mass flow rate for maximum H2 production in continuous operation. Notably, the approach contributes to mitigate adverse environmental effects associated with fossil fuel use, leveraging recycled aluminum – an abundant global waste. In essence, the herein sustainable, in situ production of green hydrogen places the hydrogen generation & fuel cell system technology in the category of a clean energy source. Therefore, the system is expected to be applicable to electric vehicles, all electric ships and stationary distributed power generation.

Biography:

José Viriato Coelho Vargasis a Mechanical Engineer, Biologist and PhD in Mechanical Engineering from Duke University, USA. He is a Full Professor at the Department of Mechanical Engineering at Federal University of Paraná, UFPR, Curitiba, Brazil, and a Visiting Professor at the Department of Mechanical Engineering and the Center for Advanced Power Systems at Florida State University, USA. He is the Chief Editor for the Thermal Engineering journal of the Brazilian Society of Mechanical Engineering and Sciences. He has published 156 JCR journal articles, 1 book, 12 book chapters, 339 conference articles and 48 abstracts, ISI H-factor: 27.

ThermoChemical Dehydrogenation of Liquid Organic Hydrogen Carriers using Innovative Catalyst Technology

Deepali Arora1*, Matt Richards1 , Julia Krstina1 , Xingdong Wang1 , Zongli Xie1 , Stuart Littler1 , Ivan Martinez-Botella1 , John Chiefari1 , and Christian Hornung1

1FloWorks Facility - CSIRO Manufacturing, Australia

Abstract:

Carriers containing chemically stored hydrogen offer an excellent pathway to bind hydrogen for safer storage and transportation, and for clean fuel generation. Therefore, hydrogen carriers such as ammonia and LOHCs are receiving significant interest in development of alternate technologies for optimal hydrogen storage and generation. CSIRO has developed a new structured catalyst platform that can be used for hydrogen generation from these carriers in a robust and efficient manner. These 3D-printed catalytic scaffolds or Catalytic Static Mixers (CSMs) offer several advantages of over conventional catalyst packed bed systems (PBS) in that they offer negligible pressure drop, predictable and tunable flow field, and the metallic scaffold offers efficient heating and improved catalyst performance. Thus, these CSMs act as great technological alternative to conventional catalyst systems for hydrogen reforming at high temperature/pressure. A novel 3D scaffold, coated with the catalyst of choice, is used for the thermochemical dehydrogenation of the substrate (aka H2 carrier). The experiments are performed inside a tubular flow reactor, under high temperature/pressure conditions. Sample analysis is performed using 1H-NMR or gas chromatography to identify process efficiencies. This work will involve investigating the influence of process parameters on reaction kinetics and comparison of CSM technology with PBS. Initial experiments show promising conversions in the system using CSMs (~55% for LOHCs and >99% for ammonia) which shows the potential of the CSM technology in hydrogen generation. Through further design and process optimization, it can serve as a robust alternative to conventional catalyst systems.

Biography:

Deepali Arora is a Postdoctoral Chemical Engineer at CSIRO (Melbourne). Her work on Hydrogen Generation using Catalytic Static Mixers is a key project under CSIRO's Hydrogen Industry Mission. She holds a Masters in Nanotechnology from Amity University and a PhD in Chemical Engineering from Curtin University. Her PhD was focused on re-engineering active pharmaceutical ingredients using dense gas processes on a microfluidic chip. She has experience in flow chemistry and microreactor technology for sensing and manufacturing applications. Her research interests include flow chemistry, microreactors, hydrogen, liquid organic hydrogen carriers, catalysis, and high temperature-high pressure processes.

Selective and Long-Lived Single Component Heterogeneous Ethylene Trimerization Catalysts Enabled by Surface Lithiation

Uddhav Kanbur[1]*, Jacklyn N. Hall[1], Yu Lim Kim[1], A. Jeremy Kropf[1], Cong Liu[1], Massimiliano Delferro[1], David M. Kaphan[1]

[1]Argonne National Laboratory, USA

Abstract :

Homoleptic chromium alkyl complexes have been immobilized on anatase titania (TiO_2) nanoparticles as well as on silica to produce $\mathbf{1}^{TiO2}$ and $\mathbf{1}^{SiO2}$ respectively. Treatment of these materials with n-butyllithium led to the reduced chromium complexes $\mathbf{1}^{LTO}$ and $\mathbf{1}^{Li/SiO2}$. The set of heterogeneous complexes were studied in detail X-ray absorbance spectroscopy (XAS), electron paramagnetic resonance (EPR) and SQUID magnetometry. Reactions with ethylene were conducted at ambient as well as at elevated pressures and product distributions were analyzed by gas chromatography and NMR spectroscopy. $\mathbf{1}^{LTO}$ converts ethylene to hexenes with a high selectivity (>80%), sustained over long reaction times at elevated temperatures. Furthermore, the exclusive formation of C_4 and C_6 olefins without a statistical (Flory-Schulz) distribution is indicative of an oxidative cyclization mechanism rather than the traditional Cossee-Arlman mechanism and indicates a uniform, single-site chromium catalytic center. $\mathbf{1}^{Li/SiO2}$ converts ethylene to polyethylene as well as short chain oligomers, suggesting mixed active sites. On the other hand, the unreduced chromium catalysts exclusively provided ultra-high molecular weight polyethylene. Partial lithiation of $\mathbf{1}^{TiO2}$ also provided a method to control rates and chemoselectivity of the ethylene reaction, and a crossover from the polymerization to oligomerization regime was observed at a 10% Li intercalation.

Biography:

Education:

- PhD, Inorganic Chemistry, Iowa State University, 2022
- BTech, Chemical Technology, Institute of Chemical Technology, Mumbai, India, 2016

Uddhav's primary area of research is surface organometallic chemistry and its application in catalysis and polymer upcycling.

A Thermally Stable Ru Catalyst: The Effect of Dandelion Rutile Support for Selective CO methanation

aDepartment of Physics and Engineering Science, Coastal Carolina University South Carolina

bMolecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Johannesburg, RSA

The possible commercialization of proton exchange membrane fuel cells (PEMFC) depends on reducing the concentration of CO in the reformate gas through viable methods [1,2]. Different rutile morphologies were applied in selective methanation as an alternative technique for the removal of trace CO concentration from reformate gas for fuel cell applications. A novel methanation catalyst in the form of Ru supported on a rutile dandelion-like structure showed a relatively higher surface area than Ru supported on a thermally produced rutile catalyst. The dandelion-like supported Ru (prepared by both impregnation and deposition precipitation by urea) revealed a superior catalytic activity over the thermally produced rutile supported catalyst in both only CO methanation and in the presence of excess CO2. Almost similar CO conversions were recorded for both P-25 and dandelion-like supported catalysts. Characterization studies involved the use of in situ powder X-ray diffraction and proved to be sinter resistant an indication that they are very well suited to high temperature use.

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2. E.D. Park, D. Lee, H.C. Lee, Catal. Today 139 (2009) pp. 280-290.

David Kumi: Ph.D. in Material Engineering (2016); MSc. in Materials and Metallurgical Engineering (2011): University of the Witwatersrand, South Africa. Research fellowship: Korea Institute of Science and Technology. Research interests: heterogeneous catalysis based on designing nanomaterials with distinct architectures, such as titania nano dandelions, and designing functional energy-efficient nanomaterials with applications in quantum dot LED (QLED) and solar cell devices. David authored and co-authored several articles in high impact factor journals such as Applied Catalysis B (19.6), ACS catalysis (12.6). He joined CCU 2021 as a faculty and laboratory manager for the engineering materials program.

Benefits and Scaling Methods for Atomic Layer Deposition Enhanced Catalysts

Julian Edwards

Forge Nano Inc, Thornton, CO

Abstract Not Available!!!!

Linker-Dependent Stability of Metal-Hydroxide Organic Frameworks for Oxygen Evolution

Daniel J. Zheng,[1,#,*] Mikaela Görlin,[2,3,#] Kaylee McCormack,[4] Junghwa Kim,[2] Jiayu Peng,[1] Hongbin Xu,[1] Xiaoxin Ma,[5] James M. LeBeau,[1] Roland A. Fischer,[5] Yuriy Román-Leshkov,[4] Yang Shao-Horn[1,2,6]

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[#]These authors contributed equally.

Abstract:

Metal hydroxide organic frameworks (MHOFs) are a new class of oxygen evolution reaction (OER) catalysts consisting alternating layers of metal hydroxides with aromatic linkers.[1] However, similar hybrid inorganic-organic hybrid materials, such as metal organic frameworks (MOFs), have proven to be unstable during OER.[2] We investigated Ni-based MHOFs with different π-π stacking energies to understand how this difference affects the morphological, structural, and transformation rate of MHOFs during OER in basic electrolytes.[3] All MHOFs were observed to undergo significant activation during cyclic voltammetry, with two orders of magnitude increase in OER activity after 18 hours. Using high-resolution microscopy and in situ spectroscopy techniques, $NiOOH_{2-x}$ was identified as the OER active phase, where a strong correlation between the dissolution of linkers from the MHOF structure with the number of electroactive Ni sites was observed. As the turnover frequency showed little change with cycle number, the enhanced OER activity is attributed to the increased number of electroactive Ni sites with cycling due to linker loss. We propose a transformation scheme from the MHOF phase to $NiOOH_{2-x}$-like phase where mono-μ-oxo motifs present only in MHOFs convert to di-μ-oxo motifs of a $NiOOH_{2-x}$-like phase. The transformation rapidly occurs in MHOFs with weaker π-π stacking energies, while stronger π-π confine the changes to the near-surface regions. This work provides valuable insights into the driving force for the chemical transformation of M(H)OFs to oxyhydroxides under electrochemical conditions and highlights the importance of linker selection for the design of highly active, yet stable, M(H)OFs for electrochemical applications.

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2. Zheng, W., Lee, L. Y. S. Metal-Organic Frameworks for Electrocatalysis: Catalyst or Precatalyst? *ACS Energy Lett.* 6, 2838–2843 (2021).
3. Zheng, D.J., Görlin, M. *et al.* Linker-Dependent Stability of Metal-Hydroxide Organic Frameworks for Oxygen Evolution. *Chem. Mater.* 35, 5017-5031 (2023).

Biography:

Daniel Zheng is a PhD student in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology, advised by Prof. Yang Shao-Horn and Prof. Yuriy Román-Leshkov. His research is focused on the design and characterization of electrocatalysts for the production and utilization of liquid fuels by connecting structure-property relationships of emerging catalyst classes (metal organic frameworks, high entropy-alloys, etc.) to develop new descriptors.

Metal catalyst-dependent poisoning effect of organic sulfur species for the hydroconversion of 5-hydroxymethylfurfural to liquid biofuels

Aleksei Turkin*, Ekaterina Makshina, Bert Sels

KU Leuven, Belgium

Abstract:

5-Hydroxymethylfurfural (HMF) is considered as an intermediate between biomass and promising liquid biofuels 2,5-dimethylfuran (DMF) and 2,5-dimethyltetrahydrofuran (DMTHF). For biofuels synthesis, noble metal catalysts are often used due to their high intrinsic hydrogenation activity and sufficient ability to perform C–O hydrogenolysis reactions. However, the catalytic performance of noble metals can be strongly affected by the presence of various compounds that can act as poisoning agents. Recently, we have reported an enormous impact of trace dimethyl sulfoxide (DMSO) impurities on the HMF hydroconversion product selectivity over Ru/C. DMSO was able to modify active sites for furan ring hydrogenation resulting in dominant DMF formation instead of DMTHF formation with pure HMF (selectivity shift from 76% DMTHF to 93% DMF). Nonetheless, we lacked a deeper understanding of the mechanism of DMSO poisoning effect and its applicability to alternative catalytic systems.

In the present study, HMF hydroconversion over commercial noble metal catalysts in the presence of various sulfur species, including DMSO, was therefore investigated. The presence of DMSO affected ring-saturated product selectivity for the metal catalyzed reactions using molecular hydrogen, whereas it fully deactivated catalytic transfer hydrogenation in 2-propanol. This shift in selectivity was due to the formation of sulfide/thiol groups on the catalyst surface. Moreover, the degree of this effect correlated with thermodynamic favorability of metal sulfide formation. To overcome the sulfur poisoning, we proposed DMSO removal with organic solvent extraction and catalyst oxidation post-treatment. These findings pinpoint the crucial role of the biobased HMF purity for reductive catalytic studies.

Biography:

Aleksei Turkin obtained his MSc in Chemistry at the Lomonosov Moscow State University (laboratory of Kinetics and Catalysis) in 2018. Upon graduation, he joined the group of Prof. Bert Sels and started a Ph.D. which was focused on biomass-derived HMF valorization during its reductive catalytic conversion. After obtaining his Ph.D. degree in 2023, he continues his research work as a post-doctoral researcher in the group of Prof. Bert Sels, where he explores the production of sustainable aviation fuels from carbohydrate feedstock.

The End

Oral Presentation

Cascaded Compression of Size Distribution of Nanopores in Monolayer Graphene for Advanced Separation Membrane

Jiangtao Wang

Massachusetts Institute of Technology, Cambridge, MA

Abstract Not Available!!!

Novel Fluorescent α-Amino Acids for Bioimaging in Living Systems

Department of Chemistry and Biochemistry, and UMass Cranberry Health Research Center, University of Massachusetts Dartmouth, Dartmouth, MA 02132, USA

Abstract :

Incorporation of fluorescent amino acid probes as a mechanism to track protein function, transport, and folding is a partivular interesting aera in chemicl biology. Recently, we and others have been developing a novel technology for real-time protein imaging in living systems via genetically encoded incorporation of an unnatural fluorescent amino acid (FAA) probe into a protein of interest. Creating novel FAAs with varied fluorescent wavelengths is a key part to achieve this challenging goal. We have recently developed a new synthetic strategy to create new FAAs via a facile coupling of fluorescent dyes to the side chain of L-phenylalanine, creating a series of novel fluorescent α-amino acids that emits blue and bright cyan fluorescence. Moreover, we have also developed a novel photochemistry method to create L-Leucine or L-methionine-based FAAs emitting in green wavelengths. These novel FAAs showed excellent photo property, bioavailability and bioimaging capabilities in cell models and animal models, representing a novel class of biomaterial for protein bioimaging in living systems. We thank UMass Dartmouth for a seed grant.

Biography:

Dr. Guo received his Ph.D. from Edinburgh University, UK and postdoctoral training at University of California Irvine. He established his independent research laboratory in University of Massachusetts Dartmouth in 2004. He is currently a full Professor in Chemistry and Biochemistry, and founding Director of UMass Cranberry Health Research Center. Dr. Guo's research interest is at the interface of chemistry, biology, and medicine, with numerous publications and patents. Dr. Guo serves as an editor of a few scientific journals and was named an IAAM Fellow in 2020.

Advancing Environmental Chemistry through Intelligent Coordination Polymers in the Remediation of Harmful Volatile Organic Compounds

Elisabete C.B.A. Alegria

Universidade de Lisboa, Portugal

Abstract Not Available!!!

Chemo-Enzymatic Synthesis of Enantiopure Vasodilator (–)-Nebivolol

Elisabeth Egholm Jacobsen,[1]* Sara Aasen[1] and Petter Daleng[1]

[1]Department of chemistry, Norwegian University of Science and Technology, Høgskoleringen Trondheim, Norway

Abstract :

The American Heart Association reported in March 2019 their update on heart diseases and stroke statistics. The report states that the prevalence of high blood pressure in the United States between 2013-2016 was 46% of the total population at ages 20 years and older. It was the cause of death for 82,735 Americans in 2016 and costed the American society approximately $ 55.9 billion in the period 2014-2015 [1]. A class of drugs that have been used both in cardiovascular and non-cardiovascular treatment are the β-adrenergic blocking agents (betablockers). This class of drugs were introduced into clinical medicine in the early 1960's, and since then, the findings of these drugs have led to a discovery of the importance of the sympathetic nervous system in the pathophysiology of a wide variety of cardiovascular and non-cardiovascular disorders [2]. We have for some time developed efficient chemo-enzymatic protocols for synthesis of several betablockers [3a-e]. Here, we present our protocol for the enantiopure vasodilator (–)-Nebivolol, fig. 1. Due to the four stereogenic centra in the molecule there are 16 possible isomers when no catalysts is used in the synthesis. However, due to symmetry, there are 10 possible isomers. We have achieved to produce the (*R*,*S*,*S*,*S*)-nebivolol.

Biography:

Elisabeth E. Jacobsen completed her MSc in Organic chemistry 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 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.

Structure-property-activity relationship of alumina supported bimetal catalysts for low-temperature total catalytic oxidation of organic air pollutants

Nataša Novak Tušar,[1,2]* Tadej Žumbar[1], Petar Djinović[1,2], Nataša Zabukovec Logar,[1,2]

[1]National Institute of Chemistry, Slovenia; [2]University of Nova Gorica, Slovenia

Abstract :

Volatile organic compounds (VOCs) are the main class of air pollutants, emitted from various industrial processes. Catalytic oxidation is one of the most important processes for removing of low concentration volatile organic compounds (VOCs) from industrial waste gases. Transition metal nanoparticles immobilized on a suitable support are low-cost alternative to currently used noble metal-containing catalysts. A synergistic effect was observed in some cases over bimetallic transition metal catalysts that enhanced their total oxidation activity at lower temperature in comparison to monometallic ones. To study the mentioned phenomenon, affordable and scalable Fe-functionalized γ-alumina was prepared via direct synthesis followed by deposition of Cu. The material was tested as catalyst in total oxidation of toluene as volatile organic compound (VOCs). The nature of the metal-support bonding and the optimal abundance between Cu-O-Al and Fe-

O-Al species in the catalysts is the reason for the synergistic catalytic activity which is promoted by small amounts of iron (Fe/Al= 0.005). The change in the metal oxide-cluster alumina interface is related to the nature of the surfaces to which the Cu atoms attach. The oxidation of toluene occurs via Langmuir-Hinshelwood mechanism. The CuFeOx/γ-alumina catalyst surpasses the benchmark activity of CuMnOx/γ-alumina catalyst in the temperature range of 300–380°C. Understanding the structure-property-activity relationship of the designed bimetallic oxide catalysts on γ-alumina support is extremely important not only for the described targeted application for air pollution prevention, but also for other applications in heterogeneous catalysis, green chemistry, advanced manufacturing, and furthermore in electrocatalysis and photocatalysis.

Biography:

Prof. Dr. Nataša Novak Tušar has been the head of the Laboratory for Catalysts at the Department of Inorganic Chemistry and Technology at the National Institute of Chemistry in Ljubljana since 2020. Since 2018 she has been a full professor and director of the PhD program "Materials" at University Nova Gorica, Slovenia. After obtaining her PhD in Chemistry, she was Individual Marie Curie Fellow at the synchrotron ELETTRA and at the University of Trieste, Italy, from 2003-2004. She is a member of the governing bodies of ENMIX (European Nanoporous Materials Institute of Excellence) and EFCATS (European Federation of Catalysis Societies).

Role of catalyst in toluene side chain alkylation with methanol – An industrial perspective

Kartick Mondal[1]*, Rikesh Joshi[1], Sandeep Negi[1], Jagadeesh Matolli[1]

[1]Shell Technology Centre, Bangalore, India

Abstract :

Ethylbenzene (EB) is an important captive intermediate for Shell. EB is currently produced by the reaction of benzene and ethylene through the EBSM process. In the mid-sixties, Sidorenko et al. [1] reported high selectivities to styrene and ethylbenzene in the alkylation with methanol of toluene performed over moderately basic X zeolites with a low Si/Al ratio. The side chain methylation reaction of toluene receives a lot of attention, since a) it has theoretical potential as a novel route to styrene b) This process is thermodynamically nearly zero (net heat of reaction), when the rates are properly balanced: methanol dehydrogenation yielding formaldehyde is endothermic while the reaction of toluene and formaldehyde is exothermic [2] & c) feedstock price advantage compared to the conventional route. For the successful deployment of this technology, it is important to reach the steep performance targets which in turn requires a better understanding of the underlying reaction mechanism and pathways to the products (both desired and undesired) where catalyst plays a very important role.

In this talk I will focus on technology maturation journey of Shell's R & D program with taking the example from one such project.

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2. Shreiber, E.H.; Rhodes, M.D.; Roberts, G.W. Appl. Catal. B: Environmental 1999, 23, 9

Acknowledgments:

D.G. Lahr, J. Zhang, M.K. Pendyala, S. Ganji

Biography:

Dr. Kartick Mondal has over 19 years of experience in Chemistry & Catalysis. He completed his PhD in Chemistry from National Chemicals Laboratory (NCL), Pune. Following this, he did two Post-docs, in University of Witwatersrand, Johannesburg, South Africa & was with RWTH-Aachen University, Germany. He was recipient of prestigious Alexander von Humboldt fellowship. He joined SABIC Research & Technology, India & worked for 6years in the area of catalyst innovative ideation and progressed several ideas through the early stage of the innovation funnel. His work with the assets on understanding dehydrogenation catalyst deactivation phenomena was instrumental in demonstrating savings for business. He joined Shell in 2015 & his focus was on primarily on leading Ideation, & business sponsored R & D programs. His technical accomplishments include 30 peer reviewed international publications, 6 granted patents, 1 Book Chapter & lead author of 20+ Shell internal reports.

On the personal front, he lives with his wife (Sudeshna) and his daughter (Labannya) & enjoys spending time with family & friends, playing badminton, Cycle riding and long-distance driving.

Large-scale simulations of catalytic surface dynamics with first principles machine learning

Boris Kozinsky

Harvard University, USA

Abstract :

Understanding atomic-level processes in surface science and heterogeneous catalysis is complicated by the wide range of time scales and length scales needed for simulations. We obtain Insights into atomistic structures and restructuring mechanisms in surfaces and nanoparticles using interdisciplinary collaborative approaches combining the use of first-principles computations, machine learning, reactivity measurements, and spectroscopy. We investigate mechanisms of surface reconstruction of noble metals, nanoparticle shape changes due to reactive conditions, and identify reactive sites of bimetallic catalysis using direct reactive MD simulations.

To accelerate molecular dynamics calculations, we rely on machine learning methods to capture interatomic interactions with quantum accuracy. We then implement and deploy these models on parallel GPUs to reach billions of atoms in size or microseconds in time. One method is a family of equivariant interatomic potential models (NequIP and Allegro) based on symmetry-preserving layer architectures that we use to achieve state-of-the-art accuracy and training efficiency for simulating atomistic. Another method (FLARE) enables autonomous selection of training sets for reactive systems, based on adaptive closed-loop algorithm that constructs accurate and uncertainty-aware Bayesian force fields on-the-fly from a molecular dynamics simulation. We examine the current limitations of machine learning models and highlight the usefulness of ML-accelerated MD simulations to study surface reconstruction, direct heterogeneous reactions, and nanoparticle shape changes.

Biography:

Boris Kozinsky studied at MIT for his B.S. degrees in Physics, Mathematics, and Electrical Engineering and Computer Science, and received his PhD degree in Physics also from MIT. He then worked at Bosch Research where he established the atomistic computational materials design team. In 2018 he started a group at Harvard University, that develops computational and machine learning methods and uses them for understanding electronic and atomistic mechanisms of transport, phase transformations and reactions in materials.

Modification and Doping of Colloidal Nanoparticles by Laser Post-Processing With Single Laser Pulses

Sven Reichenberger1 , Dana Krenz1 , Kinran Lau1 , Joachim Landers2 , H. Wende2 , Stephan Barcikowski1

1Technical Chemistry I & Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen

2Faculty of Physics & Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen

The availability and development of high performance nanocatalysts with designed functionality and durability is one of the backbones for a successful transition towards a renewable but also economic energy and chemical industry sector. In particular, nanoscale surface features such as dopants but also point, line, planar, or bulk defects contribute significantly to their catalytic activity and selectivity, making precise control of such structural features important for a tailored material design. In turn, sufficient material masses are required to use the respective nanomaterials in catalytic applications. As will be presented in this talk, we have established a continuously operating laser postprocessing of colloidal nanoparticles that allows us to imprint surface-near defects and dopants while maintaining the particle BET surface area, phase purity and shape with considerable throughput. [1]–[3] As will be shown at the example of TiO2 nanoparticles that were laserprocessed in water, the density of oxygen vacancy defects as well as the density of bridging hydroxyl groups increased linearly with each employed laser pulse.[4] Within our previous study we have further shown that fluoride ion substitution at different pH-values is a versatile tool to quantify the density and probe the acidity/basicity of surficial hydroxyls.[4] Recent results presented will also demonstrate the general applicability of this fluoride substitution to other oxides beyond TiO2. In the second part of this talk, the focus will shift to spinel-type ferrites (e.g. CoFe2O4), where nanoparticle post-processing with single laser pulses has so far allowed us to tailor the cation occupancy of tetrahedral and octahedral sites probed by Mössbauer spectroscopy and the inversion parameter, respectively.[2] As part of an ongoing laserprocessing study using other ferrites with a selection of initial cation occupancies, we intend to generalize the observed trends of the cation occupancy to mechanistically understand how the cation mobility during laser-induced heating on ns-timescale and the employed laser fluence affects the final nanomaterial structure.

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NEW CATALYTIC SYSTEMS OF FOR HYDROBORATIONS OF UNSATURATED FEEDSTOCKS

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2University of Barcelona, Spain;

3University of Bologna, Italy

Abstract :

The hydroboration of unsaturated feedstocks has emerged as a pivotal process in modern synthetic chemistry, facilitating the synthesis of valuable organoboron compounds. Organoboron compounds play a pivotal role as intermediates, offering pathways for transformations involving C–B bonds to evolve into C–C and C–N bonds via a myriad of methodologies. An efficient and widely applicable approach is the hydroboration of alkenes and alkynes, which utilizes cost-effective precursors and expeditiously provides both linear and branched organoboron derivatives. This research initiative is dedicated to pioneering novel catalytic systems, centered around rhodium (Rh) and cobalt (Co) catalysts, with the aim of expanding the horizons of hydroboration reactions. This expansion is particularly focused on embracing a broader array of unsaturated substrates, especially those abundantly available within the petroleum industry. At the core of this project lies the pursuit of innovative, efficient, and dependable catalytic asymmetric methodologies. This undertaking encompasses the entire spectrum of catalyst development, encompassing design, synthesis, and practical application. A defining facet of this work involves the construction of catalysts with modularity in mind. This modularity is achieved through versatile preparatory techniques, incorporating both organic and inorganic transformations, as well as supramolecular processes. This approach not only facilitates finetuning of catalyst properties but also promotes adaptability across diverse substrates. Integral to the advancement of these catalytic systems is a comprehensive computational analysis of the catalytic cycles.

Biography:

Chemistry research has always been my foremost passion, a pursuit I've engaged in since earning my Chemical Engineering degree from Ghana's University of Kwame Nkrumah and Technology in 2020. I've enriched my academic foundation with practical insights garnered from diverse research roles. These experiences have deepened my understanding of industrial challenges and effective solutions. Presently, I am pursuing an MSc in Chemical Innovation and Regulation, a program jointly taught by three prestigious institutions: the University of Algarve, the University of Bologna, and the University of Barcelona.

Synthesis of α,ω-Primary Hydroxyl-Terminated Polyether Polyols Using Prussian Blue Analogues as Catalysts

ByeongRyeol Moon*, Chinh Hoang Tran and Il Kim.

School of Chemical Engineering, Pusan National University, Busandaehag-ro 63-2, Geumjeong-gu, Busan , South Korea

Abstract:

Polyalkylene oxide polyether polyols are the most frequently used raw materials for polyurethanes production. These polyols are commonly produced via ring-opening polymerization (ROP) of epoxides, notably, propylene oxide (PO). However, polyols produced by PO containing certain amount of secondary hydroxyl terminal groups which make them less reactive than those capped with primary hydroxyl groups limiting the expansion of the application like polyurethanes. We have developed a viable procedure for producing α,ω-primary hydroxyl-terminated polymers and copolymers using various Prussian blue analogues as heterogeneous catalysts and polypropylene oxide (PPO) as a macroinitiator. Accordingly, PPO polyols capped with ε-caprolactone (CL) and the PPO-PCL block copolymers were successfully synthesized via ring-opening reaction and ROP of CL. The resultant polyols exhibited great enhancement in the formation of polyurethane compared to that of conventional polyols.

Biography:

ByeongRyeol-Moon earned a Bachelor's degree in department of advanced materials chemistry from Dongguk University in 2022. He is studying on the Prussian blue analogues and the synthesis of biodegradable polyols for master under the supervision of Prof. Il Kim.

The End

Oral Presentation

Metal catalyst-dependent poisoning effect of organic sulfur species for the hydroconversion of 5-hydroxymethylfurfural to liquid biofuels

Aleksei Turkin*, Ekaterina Makshina, Bert Sels

KU Leuven, Belgium

Abstract:

5-Hydroxymethylfurfural (HMF) is considered as an intermediate between biomass and promising liquid biofuels 2,5-dimethylfuran (DMF) and 2,5-dimethyltetrahydrofuran (DMTHF). For biofuels synthesis, noble metal catalysts are often used due to their high intrinsic hydrogenation activity and sufficient ability to perform C–O hydrogenolysis reactions. However, the catalytic performance of noble metals can be strongly affected by the presence of various compounds that can act as poisoning agents. Recently, we have reported an enormous impact of trace dimethyl sulfoxide (DMSO) impurities on the HMF hydroconversion product selectivity over Ru/C. DMSO was able to modify active sites for furan ring hydrogenation resulting in dominant DMF formation instead of DMTHF formation with pure HMF (selectivity shift from 76% DMTHF to 93% DMF). Nonetheless, we lacked a deeper understanding of the mechanism of DMSO poisoning effect and its applicability to alternative catalytic systems.

In the present study, HMF hydroconversion over commercial noble metal catalysts in the presence of various sulfur species, including DMSO, was therefore investigated. The presence of DMSO affected ring-saturated product selectivity for the metal catalyzed reactions using molecular hydrogen, whereas it fully deactivated catalytic transfer hydrogenation in 2-propanol. This shift in selectivity was due to the formation of sulfide/thiol groups on the catalyst surface. Moreover, the degree of this effect correlated with thermodynamic favorability of metal sulfide formation. To overcome the sulfur poisoning, we proposed DMSO removal with organic solvent extraction and catalyst oxidation post-treatment. These findings pinpoint the crucial role of the biobased HMF purity for reductive catalytic studies.

Biography:

Aleksei Turkin obtained his MSc in Chemistry at the Lomonosov Moscow State University (laboratory of Kinetics and Catalysis) in 2018. Upon graduation, he joined the group of Prof. Bert Sels and started a Ph.D. which was focused on biomass-derived HMF valorization during its reductive catalytic conversion. After obtaining his Ph.D. degree in 2023, he continues his research work as a post-doctoral researcher in the group of Prof. Bert Sels, where he explores the production of sustainable aviation fuels from carbohydrate feedstock.

NON-OXIDATIVE DEHYDROAROMATIZATION OF LINEAR-CHAIN ALKANES ON INTERMETALLIC SURFACE

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[2]US DOE, Ames Laboratory, Iowa State University, Ames, IA, USA

Abstract:

Dehydrogenation technologies have gained significant attention industrially to produce fine chemicals. Under non-oxidative reaction conditions, these processes are typically endothermic and thus require high temperature (>600 °C). Besides, low product selectivity due to various side reactions (isomerization, cracking etc.) pose significant challenges in developing novel catalytic systems. Herein, we have demonstrated Pt-based intermetallic nanoparticles (iNPs) as a highly active and, more importantly, selective catalyst for non-oxidative dehydroaromatization of long-chain alkanes to aromatized products of benzene-toluene-xylenes (BTX) family. At a reaction temperature of 550 °C, Pt based intermetallic catalysts have shown superior activity and selectivity compared to monometallic Pt nanoparticles (NPs). For the dehydroaromatization of C6-C8 linear chain alkanes, the intermetallic catalysts yield BTX selectivity of 88, 92, and 93%, respectively. Kinetics of dehydroaromatization reaction for n-hexane, including activation energy calculations, have shown that the reaction barrier is much lower on the intermetallic surface (~ 88 kJ/mol) than the monometallic Pt surface. First-order dehydroaromatization kinetics models have demonstrated that the deactivation constant on Pt surface is one order of magnitude higher than that of the intermetallic catalysts. Furthermore, using a combination of in-situ MS analysis and rate order calculations for the dehydroaromatization of various reaction intermediates, we have developed a mechanistic understanding of the dehydroaromatization process on Pt based iNPs. These results were further supported by in-situ DRIFTS studies on Pt based intermetallics. Overall, these results have provided a platform for developing novel bimetallic catalysts for efficient and selective dehydroaromatization processes as well as provided mechanistic insights into the dehydroaromatization process of linear alkanes.

A Comprehensive Summary of the Application of Machine Learning Techniques on CO2- EOR Projects

Ganesh Thakur

University of Houston, Houston, TX

Abstract Not Available!!!

Seeing is Believing: Operando Spectroscopy Studies of the Fundamental Chemistry and Application of the Solid Oxide Fuel Cell Anode $Sr_2Fe_{1.5}Mo_{0.5}O_6$ with Renewable Biofuels

Bryan Eigenbrodt[1]*, Marissa Bradley[1], Darnell Pierre[1], Daniel White[1], Andrew D'Orazio[1], Gregory Bode[1]

Villanova University, Department of Chemistry, USA

Abstract:

Efforts to commercialize solid oxide fuel cell (SOFC) technology have moved away from hydrogen fuel due to high generation costs and challenges associated with fuel storage. Instead, SOFC development has focused on discovering new electrocatalytic materials capable of efficiently converting renewable hydrocarbon fuels into electricity and products. Coupling renewable fuels with SOFC's high conversion efficiencies, can lead to more environmentally friendly energy devices with minimal carbon footprints. However, current Ni-based anode catalysts for SOFCs, cannot operate with prolong exposures to these fuels due to the deactivation of the anode catalyst by graphite deposits. The integration of the mixed ionic and electronic conductor, $Sr_2Fe_{1.5}Mo_{0.5}O_{6-\delta}$ (SFMO), was used as an anode catalyst in the SOFC to create a device that has the potential to utilize renewable hydrocarbon fuels. The use of operando spectroscopy and electroanalytical techniques will be used to explore and understand the ability of SFMO to act as an effective anode catalyst in the presence of these complex fuels. Specifically, X-ray absorption spectroscopy and a custom-built reactor assembly will allow for the non-invasive exploration of SFMO's local electronic structure and oxide vacancy formation under reducing and oxidizing atmospheres at 800°C. In addition, Raman Spectroscopy coupled with chronoamperometry will explore fuel oxidation chemistry of alcohol over the SFMO catalyst and its ability to resist graphite formations. The combination of these advanced spectroscopy techniques with electrochemical measurements will provide unparalleled insight into the catalytic properties of SFMO and its ability to be an effective catalyst for SOFCs operating with renewable hydrocarbon fuels.

Biography:

Dr. Bryan Eigenbrodt received his Ph.D. from the University of Maryland under the advisership of Professor Robert Walker. He then went on to receive a prestigious National Research Council Fellowship to conduct his post-doctoral research within the Air Force Research Laboratory at Wright Patterson Air Force Base. The focus of this research was to develop novel fuel cell catalysts and to utilize the Advanced Photon Source at Argonne National Laboratory to perform operando studies of fuel cells. Dr Eigenbrodt now continues this research and more as an Associate Professor in the Department of Chemistry at Villanova University.

Application of Visible Light Active Immobilized Ag-TiO2 Nanoparticles for the Antibiotics Removal and Disinfection in Wastewater

N.V.M. Sri Harsha, Swatantra Pratap Singh, and Amritanshu Shriwastav*

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

Abstract:

Presence of antibiotics in water and wastewater matrices is an emerging concern due to associated environmental implications. Advanced treatments, viz. photocatalysis, are being actively investigated due to the inherent limitations of conventional treatment technologies. Similarly, the process of photocatalysis is gaining interest for water disinfection. In the present study, silver doped TiO2 (Ag-TiO2) nanoparticles were synthesized in 1:1.7 (Ag:Ti) molar ratio by sol-gel method and immobilized onto the substrate. Synthesized Ag-TiO2 catalyst was characterized by SEM-EDX, FTIR, XRD, UV-DRS, and photoluminescence analysis. Doping with silver decreased the bandgap energy of Ag-TiO2to 2.41 eV, and increased the photocatalytic activity to visible light. The efficacy of these Ag-TiO2 nanoparticles was investigated for degradation of 5 ppm Ciprofloxacin (CPX) and disinfection of 106 CFU/mL Escherichia coli (E. coli) in both slurry mode and immobilized form. After 3 hours of visible light irradiation with blue LED, ~75% CPX removal and complete disinfection were obtained in batch mode application with 0.5 g/L catalyst in slurry, while 50% CPX removal and 2-3 log E. coli removal was observed with one immobilized plate in a fountain-type reactor with continuous inner recirculation. Further modifications in the setup to provide longer contact time and increased surface area resulted in improved performance for both CPX removal and disinfection with immobilized Ag-TiO2 nanoparticles. Suitable regeneration of these catalysts was also investigated. Finally, the toxicity of the treated effluent was assessed by well diffusion method. Keywords: Ag-TiO2 nanoparticles; Ciprofloxacin; Disinfection; immobilized catalyst; Toxicity.

Biography:

Amritanshu Shriwastav completed his PhD from IIT Kanpur where he worked on AlgalBacterial 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.

Deterministic and stochastic simulations of heterogeneous catalytic reactions: an applicative example concerning selective hydrogenation of vegetable oil

Andrea Di Giuliano (Invited Speaker)[1*] and Enza Pellegrino[1], Nicoletta Cancrini[1], Katia Gallucci[1]

Department of Industrial and Information Engineering and Economics, Università degli Studi dell'Aquila,
Piazzale E. Pontieri 1 loc. Monteluco di Roio, 67100 L'Aquila (AQ), ITALY.

Abstract:

Stochastic modelling of chemical reactions (e.g.: Gillespie's algorithm, tau-leaping,) had some recent successful applications in biochemistry, whereas applications for inorganic heterogeneous reactions are quite unexplored. The traditional modelling of inorganic heterogeneous catalysis relies on procedures derived at times lacking the current computing performances of machines, e.g.: (i) Postulation of reaction mechanism, (ii) Derivation of deterministic reaction rate law, (iii) Regression of law's kinetic parameters from experimental data. Stochastic modelling of chemical kinetics was proposed as an alternative some decades ago, in principle more suitable to interpret the inherent discrete and random nature of chemical reaction mechanisms; anyway, only the current large availability of computational power made related techniques easily applicable. This research group took experimental data of heterogeneous catalytic selective hydrogenation of vegetable oil (VO) as a case of study and investigated its kinetic modelling by both deterministic and stochastic approaches. Vegetable oils (VO) can provide sustainable feedstock to substitute chemicals obtained from petrol, if some VO properties are chemically modulated, e.g., selective hydrogenation aims to maximize the content of monounsaturated fatty acid, a product of industrial interest. The performed deterministic modelling study determined that consecutive hydrogenations

of one double bond per reactive step interpreted well the experimental data with simplified pseudo-first-order rate laws, if variable selectivities are introduced. The stochastic simulations at different numbers of initial molecules allowed a multiscale analysis of the system, confirming the reliability of the chosen reaction scheme and suggesting that the experiments were in their thermodynamic limit (in statistical-mechanic terms).

Biography:

Andrea Di Giuliano. 2013: M.Sc. in Chemical Engineering (summa cum laude), University of L'Aquila; 2017: Co-Tutelle Ph.D. in Chemical Engineering, University of L'Aquila, and in Chemistry, University of Strasbourg. He is now an Assistant Professor and Lecturer at the University of L'Aquila, Italy. His subjects of interest include: (i) synthesis, characterization, experimental testing and mathematical modeling of catalytic/sorbent materials (sorption-enhanced processes, syngas cleaning, biofuels); (ii) experiments and mathematical modelling of pyrolysis and gasification of biomasses, lignite, and solid wastes; (iii) fluid-dynamic characterization of granular solids for fluidized-bed reactors.

Hydrogen spillover in tungsten oxide bronzes as observed by broadband neutron spectroscopy neutron spectroscopy

Erwin Lalik [1], Stewart F. Parker [2], Gavin Irvine [3], Ivan da Silva [2], Matthias Gutmann [2], Giovanni Romanelli [4], Kacper Druzbicki [5,6], Robert Kosydar [1] and Matthew Krzystyniak [2, *]

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[5]Materials Physics Center, CSIC-UPV/EHU, Paseo de Manuel Lardizabal 5, 20018 Donostia-San Sebas-tian, Spain;

Abstract :

Hydrogen spillover is an elusive process, and its characterization, by means of experimental probes and ab initio modelling, poses a serious challenge. In this work, the nuclear quantum dynamics of hydrogen in a palladium-decorated cubic polymorph of tungsten oxide, Pd/cWO$_3$, are characterized by the unique technique of neutron Compton scattering augmented by ab initio harmonic lattice modelling. The total neutron Compton scattering response of hydrogen is characterized in terms of the hydrogen momentum distribution. The distribution is deconvoluted under the assumption of three pools of hydrogen with distinctly different nuclear quantum dynamical behavior: (i) hydrogen-terminated beta-palladium hydride, (ii) hydrogen in acid centers (OH+ groups) on the surface of the cubic phase of tungsten oxide, and (iii) quasi-free atomic hydrogen inside the saturated hydrogen bronze resulting from the spillover process. The ab initio modelling of lattice dynamics yields theoretical predictions for the values of the widths of proton momentum distributions in the first two hydrogen pools, which allows for obtaining the contribution and the width of the momentum distribution of the quasi-free proton pool. The width of the momentum distribution, the value of kinetic energy and the effective force constant of the potential of the mean force underlying this

distribution have been obtained for the first time for the quasi-free atomic hydrogen resulting from the hydrogen spillover process.

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.

[6] Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, 90-363 Lodz, Poland.

Enhancement of the Solar Water Splitting Efficiency Mediated by Surface Segregation in Ti-doped Hematite Nanorods

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Abstract:

Hydrogen production by solar water splitting is a very attractive idea because it allows storing solar energy in the H_2 molecules using a clean method. First demonstration of water splitting was reported 50 years ago using TiO_2 as photoanode[1]. Since then, plethora of studies were reported, owing to materials chemists' infinite imagination, addressing different classes of photosensitive materials including semiconducting oxides, III-V semiconductors[2], MOF (metal-organic framework) architectures[3], ferroelectric materials[4], etc. Band engineering is often employed targeting the same single aim: enhance the efficiency of the photoelectrochemical (PEC) process, increasing thus hydrogen production efficiency.

We report here a simple band engineering approach applied to one of the most Earth abundant materials, the hematite, using Ti doping[3-6] and tuning annealing conditions: temperature and atmosphere. Enhanced PEC activity was obtained, mediated by surface states, as evidenced using electrochemical impedance spectroscopy. We found strongly enhanced photocurrent, of more than 200 %, for Ti-doped hematite photoanodes annealed under Nitrogen compared to equivalent photoanodes annealed in air[6]. The nanoscale origin of the increased photocurrent was addressed using combined XPEEM, STXM, X-rays spectro-ptychography and STEM. Shadow XPEEM alone can be used to discriminate surface and bulk contributions of the chemistry and chemical coordination. STXM complement successfully these results evidencing formation of Ti-rich clusters for photoanodes annealed in O_2-free atmosphere. Spectro-ptychography allows to better identify and isolate both spatially and chemically Ti-rich clusters. X-ray spectromicroscopies altogether were confronted with STEM measurements and DFT calculations, the results suggesting formation of pseudo-brookite clusters at the surface of the Ti-doped hematite.

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CFD-based investigation of autothermal reactor for oxidative coupling of methane (OCM): performance analysis and optimization

Sultan Alturkistani[1]*, Lei Chen[2], Ribhu Gautam[1], S. Mani Sarathy[1]

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Abstract :

Oxidative coupling of methane (OCM) is a promising route for the direct conversion of methane into valuable C_2 hydrocarbons. Despite its potential, the commercialization of OCM has faced challenges due to the exothermic nature of the process and its associated implications. This exothermicity results in a substantial increase in reactor temperature, impacting catalyst stability and altering the optimal temperature range for desired reactions, hence posing challenges for process scalability. In this study, we investigate the feasibility of employing an autothermal reactor as an effective solution to transfer excess heat to the incoming feed stream. This approach not only solves the exothermicity issue but also reduces operational costs by operating at a lower feed temperature and addressing scalability issues. A three-dimensional computational fluid dynamics (CFD) model, based on a porous media approach, was employed to evaluate the exothermicity and heat transfer of the OCM reactor. For comparison, isothermal, adiabatic, and autothermal reactors were investigated to compare their performance. To improve the accuracy of the CFD predictions, a global reaction model was refined using high throughput screening (HTS) experiments conducted with La_2O_3/CeO_2 catalysts. These experiments were performed in a process-consistent manner to obtain a reliable database covering various operating conditions. The CFD simulations provided valuable insights into the performance of the reactors, particularly highlighting the significant temperature rise in the catalyst bed region. These insights contribute to a deeper understanding of the OCM process and provide practical guidance for the design and operation of OCM reactors.

Biography:

Sultan is a Ph.D. candidate in chemical engineering at KAUST, Saudi Arabia, supervised by Prof. Mani Sarathy. Simultaneously, Sultan is working as Scientist within the research and development division of SABIC petrochemical company in Saudi Arabia. He has more than eight years of research experience in various domains of SABIC. His research focuses on studying experimental and modeling aspects of chemical kinetics for catalytic processes. He extensively employs high throughput experimentation for testing various catalysts and developing chemical kinetic models. He has authored and co-authored articles published in journals of repute. He has also authored and co-authored two patents.

Preparation and characterization of some nano oxides (vanadium pentoxide and nickel oxide) and their use in removing tetracycline from water

Ali M. Jihad[1]*, Rashed T. Rasheed[2], Thamer Adnan Abdullah[3]*

Applied Sciences Department/University of Technology, Iraq

Abstract :

Water pollution has increased in recent years with pharmaceutical pollutants, such as tetracycline pollution. This pollutant has a harmful effect on the environment, water resources, agriculture, and drinking water for humans, animals, and agriculture. This research aims to use some nano oxides (vanadium pentoxide and nickel oxide) as an adsorbent material to remove this pollutant from water. The thermal method (reflux) was used to prepare vanadium pentoxide and the autoclave method was used to prepare nickel oxide. The prepared oxides were calcined at 500°C and then characterized by several methods, including UV/Vis, FTIR, XRD, SEM, and AFM. These prepared oxides were used to remove tetracycline from aqueous solution, and these prepared nano oxides showed variation in their removal efficiency (%R and q), depending on the type of nano and its calcination temperature. Vanadium pentoxide ranked first in removal in both cases (as prepared and calcination), and the first case (as prepared) was considered the best, so it was adopted for optimal working conditions in terms of the best weight of the adsorbent material (nano), the highest concentration of the pollutant (tetracycline), the highest concentration of the detector (permanganate), the fastest stirring speed, and the best stirring time. Isotherm calculations were also performed using Langmuir and Freundlich equations

Biography:

Thamer Adnan Abdullah is a distinguished professional who earned his BSc in Chemical Engineering from the University of Technology, Baghdad, in 2004. His academic journey continued as he achieved a master's degree in Chemical Engineering in 2014 from GGSIPU, New Delhi, India. Driven by a passion for innovation, he pursued a Ph.D. in Chemical Engineering, specializing in Nano-chemistry for Water Treatment, and successfully graduated from the University of Pannonia, Hungary, in 2022. Thamer has made significant contributions to his field, with numerous publications in esteemed web of science journals, showcasing his expertise. His scholarly impact is further evidenced by an impressive h-index of 13 in Scopus.

Phytic Acid as a Low-cost, Non-toxic and Sustainable Homogeneous Catalyst: Hydrogen Production from Alcoholysis of $NaBH_4$

Sultan BUTUN SENGEL*[1], Hatice DEVECI [1]

[1]Eskisehir Osmangazi University, Turkey

Abstract:

Phytic acid (PA) as a low-cost, non-toxic and sustainable material used as a homogeneous catalyst in the production hydrogen (H_2) from $NaBH_4$ by alcoholysis. The parameters as reaction temperature, catalyst types and amount, $NaBH_4$ amount, were all investigated as factors that affect the H_2 production rate. The efficiency of the PA catalyst was investigated in the range of 10-30°C by methanolysis reaction, and its reuse was tested. Accordingly, When the hydrogen generation

rate values between 10-30°C were compared, it was concluded that the methanolysis reaction rate increased from 278 to 434 $mL.min^{-1}$. Activation parameters for the methanolysis of $NaBH_4$ with the use of PA as a homogeneous green catalyst were calculated as 10.60 $kJmol^{-1}$, 8.49 $kJmol^{-1}$, 164.60 $Jmol^{-1}K^{-1}$, for Ea, $\Delta H^{\#}$, and $\Delta S^{\#}$, respectively.

Biography:

Sultan B. Şengel completed her master's degree on "polymer and latex synthesis characterizations" in 2010 and her PhD degree on "synthesis of monomers with different hetero atom content and synthesis, characterization and applications of their nano and microparticles" in 2017 in the Department of Chemistry. Dr. Şengel started to work as an Assistant Professor in Biomedical Engineering in 2019 and is currently working as the Head of the Department. Dr. Sengel conducts research on hydrogels, cryogels, aerogels, composites, macro systems, polymeric ionic liquids and their applications in environmental, energy and biomedical fields.

BH_4^- hydrolysis on the Ag(111) and Au(111) surfaces - a DFT Study

Haya Kornweitz[1]*, Dan Meyerstein[1,2], Basil Raju Karimadom[1]

[1] Chemical Science Department and The Radical Research Centre, Ariel University, Israel

[2] Chemistry Department, Ben-Gurion University, Beer-Sheva, Israel

Abstract :

The mechanism of the catalytic hydrolysis of BH_4^- on Au(111) and Ag(111), as studied by DFT, is reported. The borohydride species are adsorbed stronger on the Au^0-NP surface than on the Ag^0-NP surface. The electron affinity of Au is larger than that of Ag. The results indicate that only two steps of hydrolysis are happening on the Au(111) surface and the reaction mechanism differs significantly from that on Ag(111) surface. These remarkable results were experimentally verified. H_2 generation is enhanced in the presence of surface H atoms. Thus, it is proposed that the BH_4^- hydrolysis and reduction mechanisms catalyzed by M^0-NPs depend considerably on the nature of the metal.

Biography:

I am an associate professor in the Department of Chemical Sciences at 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.

Enhancing Electrocatalysis through Controlled Gas-Etching: Evolving Surface Structure of Pt-Ni Nano-Octahedra

Lihua Zhang[1]*, Can Li[2], Xiaobo Chen[3], Soonho Kwon[4], William A. Goddard III[4], Guangwen Zhou[3], and Jiye Fang[2]

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13902, United States; [3]Materials Science and Engineering Program, Department of Mechanical Engineering, State University of New York at Binghamton, Binghamton, New York, 13902, United States; [4]Materials and Process Simulation Center, California Institute of Technology, Pasadena, California 91125, United States

Abstract :

A novel approach to manipulating the atomic-level composition of an electrocatalyst surface has been recently developed through controlled gas-etching techniques [1]. This study focuses on the deliberate engineering of the (111)-exposed surfaces of Pt_3Ni nano-octahedra, synthesized from a hot colloidal solution system, *via* a carbon monoxide (CO) gaseous etching process at an elevated temperature. The outcome of this process significantly enhances the catalytic activity and stability of the nano-octahedra towards the oxygen reduction reaction (ORR) in acidic media. The modified surfaces exhibit approximately 1.8-fold and 2.2-fold improvements in mass activity and specific activity, respectively. After subjecting the surface-etched Pt−Ni nano-octahedral sample to 20,000 potential cycles of durability tests, it demonstrates a mass activity of 1.50 A/mg_{Pt}, surpassing the initial mass activity of the unetched counterpart (1.40 A/mg_{Pt}) and outperforming the benchmark Pt/C (0.18 A/mg_{Pt}) by a factor of 8. Various analyses, including high-resolution transmission electron microscopic (HRTEM) imaging, high-angle annular dark-field scanning transmission electron microscopic (HAADF-STEM) imaging, HAADF-STEM energy dispersive X-ray spectroscopic (EDX) line scan and elemental mapping, and powder X-ray diffraction (XRD), were conducted to unravel the relationship between the ORR performance and catalyst surface evolution. Integration of these investigation results indicates that, during the surface etching treatment, the octahedral morphology of Pt−Ni nanocrystals was well preserved with {111} facets and ~2 atomic layers of Pt-skin on Pt_3Ni {111} facets generated through the extraction of Ni atoms. This unique Pt-Ni surface structure is identified as the origin of the improved ORR performance.

[1] *Can Li et al., Nano Lett.,* 23 (8), 3476 - 3483, (2023)

Biography:

Lihua Zhang received her Ph.D in Materials Science from Solid Atomic Imaging Division at Institute of Metal Research, Chinese Academy of Science in 2002. Dr. Zhang spent her two-year post-doc at the National Center for Electron Microscopy, Lawrence Berkely National Laboratory from 2003-2004. Since 2005, Dr. Zhang has been working as a staff scientist in the electron microscopy group at the Center for Functional Nanomaterials, Brookhaven National Laboratory. Her research interest focuses on microstructure characterization on nanoscale materials by advanced transmission electron microscopy.

Rapid Catalyst Testing at Scale Using Interchangeable, 3D-printed Catalytic Cores and Fast, Highly Uniform Inductive Heating

Barton Norton

Kontak Hydrogen Storage, Issaquah, WA

Abstract Not Available!!!

Non-linear moments modelling of metal, oxygen and hydrogen binding to metallic surfaces

Ian Shuttleworth*

School of Science and Technology, Nottingham Trent University, Nottingham, NG NS, UK

Abstract:

The adsorption energy E_{ads} of metal, oxygen and hydrogen adsorbed on a series of strained FCC and HCP transition metal surfaces has been modelled using the first four moments $\mu(1\text{-}4)$ of the clean surface *d*-states [1-2]. For compressive and tensile surface strains of between -5% and +10% the adsorption energy E_{ads} has been shown to be effectively modelled by a degree 6 polynomial expansion of $\mu(1\text{-}4)$.

The physical justification for this model is discussed in terms of the distortion of the surface d-states during bonding, and extends the effectiveness of the conventional *d*-band model which only uses first adsorption moments $\mu(1)$ i.e. the center of the surface d-band, to cases where the surface is controllably distorted. The current work discusses the changes to the width, skewness, and bimodality of the surface electronic states of the Pt-block metals under strain, and also shows the non-linear character of adsorption under strain.

Biography:

Ian Shuttleworth started his career with a PhD in Surface Physics earned at the Cavendish Laboratories, Cambridge University. He held post-doctoral positions at both the University of Nottingham and then Rutgers University, before accepting a faculty position at Nottingham Trent University.

Ian Shuttleworth's research interests lie in the field of chemical processes that occur during heterogeneous catalysis – that is, when the phase of the catalyst is different to the phase of the reactants. Broadly, investigations within his group follow the themes of surface and interfacial science, nano-chemistry and defect chemistry

Advanced Two-dimensional Materials for Electrochemical Energy Storage and Conversion

Fei Yao

University at Buffalo, Buffalo, NY

Abstract Not Available!!!

Understanding the formation of poliaromatic compounds in the interstellar space

[1]Marta Castiñeira Reis*; [2]Emilio Martinez-Núñez; [1, 2]AntonioFernández-Ramos

[1]Center for Research in Biological Chemistry and Molecular Materials (CIQUS) and Department of Physical Chemistry, University of Santiago de Compostela, 15706, Santiago de Compostela, Spain

Abstract :

Understanding the formation of PoliAromatic Hydrocarbons (PAHs) can shed light on the origin of the prebiotic Earth and even on the origin of life.[1] Unfortunately, to date, the formation of organic compounds in space is a scarcely understood area.

In this arena, automated protocols for the identification of reaction mechanisms show great potential to aid in the learning of how PAHs are formed in space. Taking advantage of the AutoMeKin [2,3] program, we have found thousands of potential paths that account for the formation of the simplest PAHs: antracene. We have not only uncovered several direct paths, for which reactants have been detected in space, but also some more indirect paths in which well-known intermediates such as benzyne or the very acetyl radical play a crucial role.

Acknowledgements

M.C.R. thanks the Centro de Supercomputación de Galicia (CESGA) for the free allocation of computational resources and the Xunta de Galicia (Galicia, Spain) for financial support through the ED481B-Axudas de apoio á etapa de formación posdoutoral (modalidade A) fellowship.

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E. Martínez-Nuñez, *J. Comput. Chem.* 39 (**2018**) 1922–1930.

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). In 2019 she moved as a postdoc to the the University of Groningen (The Netherlands). Her research focused on the mechanistic elucidation of metal catalysed processes. Currently, she is a postdoctoral researcher at the Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (Spain) where she is working on the automatization of mechanistic searches.

Understanding the Multifaceted Mechanism of Compound I Formation in Unspecific Peroxygenases through Multiscale Simulations

Prof. Ruibin Liang*, Gustavo J. Costa

Texas Tech University, USA

Abstract:

Unspecific peroxygenases (UPOs) selectively oxyfunctionalize unactivated hydrocarbons using peroxides under mild conditions, and hold great potential as biocatalysts for industrial applications. A thorough understanding of their catalysis is necessary for improving their performance. However, it remains elusive how UPOs effectively convert peroxide to Compound I (CpdI), the principal oxidizing intermediate in the catalytic cycle. Specifically, the roles of peroxide unbinding in the kinetics of CpdI formation, which is essential for interpreting existing experiments, have been understudied. Moreover, there has been a lack of free energy characterizations with explicit sampling of protein and hydration dynamics, which is critical for understanding the thermodynamics of the proton transport (PT) events involved in CpdI formation. To bridge these gaps, we employed multiscale simulations to comprehensively characterize the CpdI formation in wild-type UPO from *Agrocybe*

aegerita. Extensive free energy and potential energy calculations were performed in a quantum mechanics/molecular mechanics setting. Our results indicate that substrate-binding dehydrates the active site, impeding the PT from H_2O_2 to a nearby catalytic base (Glu196). Furthermore, the PT is coupled with considerable hydrogen bond network rearrangements near the active site, facilitating subsequent O–O bond cleavage. Finally, large unbinding free energy barriers kinetically stabilize H_2O_2 at the active site. A delicate balance among PT, hydration dynamics, hydrogen bond rearrangement, and cosubstrate unbinding collectively enables efficient CpdI formation. Our simulation results agree with kinetic measurements and offer new insights into the CpdI formation mechanism at atomic-level details, aiding the design of new biocatalysts for sustainable chemical transformations of feedstocks.

Biography:

2011	BS in Chemical Biology, Tsinghua University, China.
2016	PhD in Chemistry, University of Chicago, USA. Advisor: Gregory A. Voth
2016-2017	Postdoc, UC Berkeley, USA. Advisor: William H. Miller
2017-2020	Postdoc, Stanford University, USA. Advisor: Todd J. Martinez.
2020-Now	Tenure-track Assistant Professor, Department of Chemistry and Biochemistry, Texas Tech University, USA

Prof. Liang's research focuses on developing and employing multiscale simulation methods to understand photoactive biomolecular systems of biomedical importance. His research has deepened our understanding of the mechanism of proton transport and photochemical reactions in biomolecules and resulted in multiple publications in top journals such as PNAS and JACS.

Probing Reaction Mechanism by Operando MAS NMR Spectroscopy

Jian Zhi Hu

Pacific Northwest National Laboratory, Richland, WA

Abstract Not Available!!!

Distal Functionalization via Transition Metal Catalysis

Haibo Ge

Texas Tech University, Lubbock, TX

Abstract Not Available!!!

Preparation, characterization, and reactivity of ZnO/Cu2O/Cu(111) surface relevant for CO2 hydrogenation to methanol reaction

Mausumi Mahapatra, 1,4 Jindong Kang, 1,2 Pedro J. ramirez, 3 Rebecca Hamlyn, 1,2Ning Rui, 1 Zongyuan Liu, 1 Ivan Orozco, 1,2 Sanjaya D. Senanayake 1 and Jose A. Rodriguez1,2

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Abstract:

The precise characterization and atomic-scale understanding of the catalyst materials' physical and chemical properties are essential for the design of selective and active catalytic systems.Here, we have studied the structure, electronic properties, and reactivity of ZnO nanoparticles on the Cu2O/Cu(111) single-crystal surface using X-ray photoelectron spectroscopy (XPS) and scanning tunneling microscopy (STM). Our results demonstrate that the growth and size of the ZnO nanoparticles are strongly dependent on the Zn deposition temperature. In a set of experiments, Zn was deposited on Cu(111) or Cu2O/Cu(111) surfaces at 300 K with subsequent exposure to O2 at higher temperatures (400−550 K), which exhibited small particles of ZnO (<20 nm in size) on the surface. The deposition of Zn onto Cu2O/Cu(111) at elevated temperatures (450−600 K) in an oxygen ambient produced large ZnO islands (300−650 nm in size), which were very rough and spread over several terraces of Cu(111). XPS/Auger spectra showed that all of the preparation conditions stated above led to the formation ZnO/Cu2O/Cu(111) surfaces where the oxidation state of zinc was uniform. Catalytic tests showed that all these surfaces were active for the hydrogenation of CO2 to methanol, but only the systems prepared at 600 K displayed longterm stability under reaction conditions. Our results establish the "structure-property" relationship which is essential for the rational design of novel catalytic materials Mausumi Mahapatra is an assistant professor of chemistry at Loyola University Chicago since the fall of 2022. She received her Ph.D. from the University of Wisconsin Milwaukee followed by postdoctoral studies at Brookhaven and Pacific Northwest National Laboratories. Her research interest focuses on heterogeneous catalysis and chemical reactions on well-defined surfaces of oxides and metal/oxide interfaces.

Study of Electrically Switching of Spin in Spin Crossover Molecules

Ruihua Cheng*

Department of Physics, Indiana University Purdue University Indianapolis (IUPUI), Indianapolis, IN, USA

Abstract :

Using spectroscopy and electric transport characterization, it is evident that the spin state of the spin crossover molecular complex [Fe$\{H_2B(pz)_2\}_2$(bipy)] (pz = tris (pyrazol-1-1y)-borohydride, bipy = 2,2'-bipyridine) depends on the ferroelectric polarization of an adjacent thin film of the polymer ferroelectric polyvinylidene fluoride-hexafluoropropylene (PVDF-HFP). The UV-Vis spectroscopy reveals that room temperature switching of [Fe$\{H_2B(pz)_2\}_2$(bipy)] molecules in bilayers of PVDF-HFP/[Fe$\{H_2B(pz)_2\}_2$(bipy)] as a function of ferroelectric polar polarization. The electric polarity dependence of bilayers of PVDF-HFP/[Fe$\{H_2B(pz)_2\}_2$(bipy)] shows a strong dependence on the thickness of the PVDF-HFP layer. The PVDF-HFP/[Fe$\{H_2B(pz)_2\}_2$(bipy)] interface may affect polarization retention in the PVDF-HFP thin film limit.

Biography:

Ruihua Cheng is currently working at the Department of Physics of Indiana University-Purdue University-Indianapolis (IUPUI) as an associate professor. She received her Ph.D in Physics at

University of Nebraska-Lincoln in 2002. Then she conducted her postdoctoral research in the magnetic thin film group of materials science division at Argonne National Laboratory. In 2005, she joined the Department of Physics at IUPUI. Her current research is focused on molecular magnetic materials characterization, particularly spin crossover molecular manipulation and their applications in molecular based devices.

Industrially-important Biocatalysts from Extreme Environments in Trinidad

Sephra Rampersad

The University of the West Indies, Trinidad and Tobago

Abstract Not Available!!!

Density Functional Theory Calculations of the thermochemistry of the dehydration of 2-propanol

Eugene Mananga[1*] , Aissata Diop[3] , Paulin Dongomale[4] , Fambougouri Diane[5] , and Hubertus van Dam2

[1]The City University of New York, USA; [2]Brookhaven National Laboratory, USA; [3] Smith College, USA; [4]Missouri University of Science & Technology, USA; [5]Tufts University, USA

Abstract :

Electronic structure theory provides a foundation for understanding chemical transformations and processes in complex chemical environments. This presentation is on the understanding of the dehydration of 2-propanol over a zeolite catalyst using the density functional theory (DFT) calculations. We investigated and analyzed the thermochemistry calculations of the dehydration of 2-propanol. Modeling computational challenges of the reaction in this study properly requires simulations using extended atomistic models. The computational outcomes of 2-propanol are validated by comparing the predictions against the dehydration of 1-propanol. The first-principles DFT calculations is used to examine the enthalpy of the 2-propanol reaction and computed the energy for geometry optimization for increasingly better basis sets: cc-pVDZ, cc-pVTZ, cc-pVQZ, cc-pV5Z, & cc-pV6Z. The various transition states and minima along the reaction pathway are critical to inform the NWChemEx science challenge calculations. The presentation explains how the accuracy of the calculations depends on the basis sets, and what basis sets are needed to achieve sufficient accurate results. We also present the calculated results of the reaction free energy as a function of temperature as thermodynamic parameter. The results presented show how the enthalpy of each basis set decreases as the number of valence orbitals increases. This work opens ways to understand how DFT can be used for the removal of water from organic compounds (2-propanol) to form new chemicals over zeolite catalysts. Further insights into catalytic properties could be obtained in the future by comparing DFT calculations to other corresponding methods of predictions.

Acknowledgements:

This research was supported by the Exascale Computing Project (17-SC-20- SC), a collaborative effort of two U.S. Department of Energy organizations (Office of Science and the National Nuclear

Security Administration) responsible for the planning and preparation of a capable exascale ecosystem, including software, applications, hardware, advanced system engineering and early testbed platforms, in support of the nation's exascale computing imperative.

Biography:

Mananga is a Professor of Physics at The City University of New York, an Adjunct Professor of Applied Physics at New York University, and a Visiting Scientist at Brookhaven National Laboratory. His research spans a range of topics in condensed matter physics, materials science, and computational science. Specifically, his research focused on controlling the spin dynamics in solid-state nuclear magnetic resonance (NMR) and using computational methods based on density functional theory to investigate and characterize materials systems for energy storage as well as zeolite catalysis. He has published more than 70 peer-review scientific articles and is the recipient of several distinguished awards including the 2018 DISTINGUISHED SCIENTIST AWARD from the American Chemical Society (New York Section) for "Contributions and Advanced Studies in the Theory of Spin Dynamics in Solid-State NMR and Quantum Mechanics."

Fabrication and characterization of visible-light-driven core-shell TiC-TiO2 nanoparticles

Sujun Guan[1],* and Yingda Qing[1]

[1]Tokyo University of Science, Japan

Abstract :

TiO2 photocatalysis has received much research interest, but the applications of TiO2 nanoparticles (NPs) as photosensitizing agents in the attention should be paid to the last mentioned, but exceptional category containing metallic and treatment of cancer as well as in photodynamic inactivation of antibiotic-resistant bacteria. However, the relative wide band gap of TiO2 and fast recombination of photogenerated charge carriers limit its overall photocatalytic efficiency. To apply TiO2 to treat cancer, it needs to make TiO2 respond to visible light and even near-infrared light, simultaneously, reduce the recombination of electrons and holes as much as possible. Presently, we had successfully fabricated core-shell TiC-TiO2 NPs (Fig. 1), with oxidizing the outer TiC to C-doped TiO2 to narrow the band gap of TiO2, and controlling the thickness of TiO2 formed on TiC NPs to reduce the recombination of electrons and holes. Results show that the photocatalytic activity of core-shell TiC-TiO2 NPs has been significantly enhanced, with encompassing the increased visible-light response caused by narrowed band gap around via C-doped TiO2, and the effect of charge transfer between TiC and TiO2.

Biography:

Guan is an associate professor working in the Photocatalysis International Research Center at Tokyo University of Science from August 2023, focusing on visible-NIR-driven photocatalysis and their environmental and bio application. Prior to this, he worked at Tokyo University of Science from April 2017 and Toyo University from April 2021, researching on the visible-driven photocatalysis, p-type ZnO semiconductor films and their related devices. Before the work, he gained his PhD from Chiba University, working on enhancement of visible-light absorption and photocatalytic activity of photocatalyst coatings.

Lignin-derived carbons for electrocatalytic applications

Izabela I. Rzeznicka[1], Alicja Klimkowicz[1], Harison Rozak[1], Hideyuki Horino[2]

[1]Shibaura Institute of Technology, Japan; [2]Tohoku University, Japan

Abstract :

Novel technologies leading to efficient conversion of biomass into energy and value-added products are being sought to achieve decarbonization goals. Lignin is the most abundant natural polymer after cellulose. Currently, most of the lignin is burnt to generate heat and power which results in the emission of large quantities of carbon dioxide into atmosphere. Lignin-derived carbons could substitute fossil fuel-based carbon black widely used as conductive additive in many technological processes. In this presentation, we will report on the properties of kraft lignin-derived carbons and their application in formulation of catalytic inks for electrocatalytic applications. In particular, we will discuss the effect of pyrolysis parameters on the physico-chemical properties of the obtained carbon dust.1)

1) This work was supported by JST Strategic International Collaborative Research Program (SICORP), Grant Number JPMJSC2302, Japan.

Biography:

Izabela Rzeznicka studied heterogeneous catalytic 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.

Well-arrayed ZnO nanrods prepared by chemical bath deposition and its catalytical activity

Chaoyang Li*, Tomoya Ikuta and Htet Su Wai

Kochi University of Technology, Japan

Abstract :

Recently, ZnO-based nanostructures have attracted much attention as photocatalysts for removing organic dye pollutants from water. The numerous reports have already demonstrated that the photocatalytic efficiency of ZnO was strongly influenced by the surface morphology and various ZnO nanostructures modification. In this research, the ZnO nanorods was synthesized by the chemical bath deposition (CBD) method. A mixed precursor solution of Zn (NO3)2·6H2O concentration of 0.015 mol/L and hexamethylenetetramine (HMTA) with a concentration of 0.0075 mol/L was prepared and dissolved in ultrapure water (200 ml) as solvent. Prepared precursor solution was poured into a flask and kept at 95 °C. The reaction time was set from 1 hour to 5 hours with one-hour interval. As the result, the crystallinity of ZnO nanorods in (0001) growth orientation was improved when the reaction time was increased from 1 hour to 5 hours during the CBD growth. When the growth reaction time was increased, more Zn2+ ions were generated and strongly bonded with oxygen. The formed ZnO crystallites could be stacked along the c-axis

(0001) growth direction resulting in the length increasing. All fabricated ZnO nanorods showed the high transmittance of over 70% in the visible region. The obtained ZnO nanorods grown with 5 hours showed the highest photodegradation efficiency and the largest value of first-order reaction rate of 0.0057 min-1. The results indicated that the obtained ZnO nanorods could be efficiently degraded the methyl red dye solution and had a high potential to be applied in photocatalyst application.

Biography:

Chaoyang Li is currently a Professor of Department of Electronics and Photonics in Kochi University of Technology, Japan. Throughout her career, Dr. Li has focus her research on the semiconductor materials with emphasis on nano-structured materials/films synthesizing and applying for dye-sensitized solar cells, gas sensors, photo catalysis and lighting, etc. She has served on the editorial boards of several scientific journals and authored over 100 publications and books. She also the senior member of Electrochemical Society, Institute of Electrical and Electronics Engineers IEEE and the Society for Information Display.

Porous organic Polymer-based Ziegler-Natta Catalysts for Propylene Poymerization

Xiong Wang* Wenqian Kang, Yue Ren, Tongsen Qiao, Guangquan Li and Yuan Xie

Lanzhou Petrochemical Research Center, Petrochemical Research Institute, PetroChina.

Abstract :

Porous organic polymers (POPs) have received increasing attentions in a wide range of areas including adsorption, separation and catalysis. In this presentation, different types of POPs were designed, synthesized and used as Zeigler-Natta catalyst support for propylene polymerization. The prepared POP could obtain highly porous structure with specific surface area of 542 m2/g (BET) and pore volume of 0.433 g/ml. The prepared POP based Zeigler-Natta catalysts with diisobutyl phthalate (ID-1) and 3-methyl-5-tert-butyl-1,2-phenylene dibenzoate (ID- 2) exhibit good propylene polymerization activity, high stereoregularity and broad molecular weight distribution. The polymerization activity of the POP-based catalysts with (ID-2) is up to 32.6 × 10^6 g.PP/mol.Ti. h with Mw/Mn of 13.8 and isotacticity index of 98.3%. The stereoregularity or isotactic sequence distribution of the prepared polypropylene (PP) was characterized by DSC、^{13}CNMR and TREF techniques, and the results showed that the POP based catalyst could obtain higher isotatic sequence than the $MgCl_2$-based Ziegler-Natta catalyst with the same internal donor. This characteristics of broad molecular weight and peculiar high stereoregularity of POP based catalyst could be attributed the modulation of chemical environment around Ti and Mg elements, and XPS analysis exhibited the minute difference of binding energy of Ti、Mg、C and O atoms. Furthermore, the plausible formation mechanism of active sites for the POP based Z-N catalyst was proposed.

Biography:

Xiong Wang was born in Hubei (China) in 1980. He received B. S. degree in chemistry (2002) and M. S. degree (2005) from Hubei University. Then he joined in Lanzhou petrochemical research center, PetroChina, focused on polyolefin catalysts and novel products. He completed his Ph. D with prof. Yanfeng Li in Polymer Chemistry and Physics (2016) from Lanzhou University. He gained the

Young Scientific and Technological Talents Award of China National Petroleum Company (CNPC) in 2018, and now he serves as a senior expert in Petrochina Petrochemical Research Institute. His research interests include Olefin Polymerization Catalysis and Porous catalytic materials.

Comprehensive Analysis of the Quality of Colloidal Gas Aphrons: Impact of Batch and Batch-recirculation Modes of Operation on Air Holdup and Stability

Isha Arora[1]*, Taybah Yousuf[2] , Faryal Malik[2] , Sameena Manzoor[2] , and Ashok N. Bhaskarwar[1]**

[1]Department of Chemical Engineering, Indian Institute of Technology, Delhi, New Delhi , INDIA

[2]Department of Chemical Engineering, National Institute of Technology, Srinagar, INDIA

Abstract :

Colloidal Gas Aphrons (CGAs) may be perceived as microbubbles with remarkable stability. Each one of these CGAs consists of an air core surrounded by a viscous hydrogen-bonded aqueous shell enveloped in an as-yet unknown number of bi-layers of surfactant. The CGAs are generated in a specially-designed baffled generator with surfactant solutions, utilizing high rotational speeds exceeding a critical value for formation, under specific experimental (geometric and hydrodynamic) conditions. CGAs serve diverse purposes. These include serving as drilling fluids and as an agent for enhanced oil recovery. Making aerated concrete, remediation of soil and water, synthesis of porous polymers, nanoparticles and porous catalysts, and targeted-drug delivery are other applications. A substantial body of literature comprehensively explores the applications of CGAs, some elucidating even their structural and dispersion features to a limited extent. These aspects are intricately influenced by a spectrum of parameters, including the nature and type of surfactant, surfactant concentration, disc rotational speed, temperature, pressure, pH, and salt concentration. Very limited understanding, however, exists regarding the variations in the properties of CGAs when generated in a recycle mode of operation of a CGAs generator. The present paper systematically explores experimentally both the batch and batch-recirculation modes to evaluate their influence on CGAs quality, specifically focusing on air holdup and stability. A meticulous examination of the effects of surfactant concentration, disc rotational speed, and CGAs recirculation rate offers valuable insights into the dynamics of formation and overall stability of CGAs. Furthermore, the anticipated distinctions between the outcomes of batch and batch-recirculation modes of operation of a CGAs generator are analyzed and discussed. Batch-recirculation demonstrates negligible influence on the air holdup and volume of CGAs generated over extended durations, yielding results comparable to those observed in batch mode. Nonetheless, a noticeable enhancement in the CGAs build-up occurs during the initial stages of the recirculation mode of operation.

Biography:

Professor Ashok N. Bhaskarwar, with a Ph.D. in Chemical Engineering from IISc, Bangalore, has been teaching at IIT Delhi since 1990. A visiting professor at the University of Minnesota, he holds 40 patents and authored 258 publications, including books. He founded EnNatura Technology Ventures Pvt. Ltd., a startup focusing on eco-friendly lithographic printing inks. As a consultant to top Indian industries, his impact extends beyond academia. Isha Arora, his Ph.D. student at IIT Delhi, is currently working on Modeling the dynamics of Colloidal Gas Aphrons generation. She has 5 publications including journal papers, conference paper, and book chapters.

Transformation of Biorenewable Sugar Feedstocks to Specialty Chemicals

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

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

Abstract:

The production of petroleum-based chemicals from renewable resources has regained attention due to rising prices of crude oil and petrochemical feedstock in recent years. Manufacturing bio-chemicals adds more value to products, allows smaller scale and is characterized by smaller capital expenditures, as compared to bio-fuels. A variety of commodity chemicals can possibly be made from biomass resulting in lower costs than state-of-art petrochemical methods [1].

We present industrially relevant transformations of low-cost sugar feedstocks into market chemicals and monomers for high-performance polymers by chemo-catalytic processes in continuous flow trickle beds. Since long term catalyst stability under hydrothermal conditions is an important issue to be addressed in liquid phase catalysis, we will primarily discuss results of catalytic performance for prolonged times on stream. In particular, a 2-step process for the production of adipic acid from glucose has been developed by Rennovia and successfully demonstrated in a pilot scale unit with all ancillary operations including solvents recovery and adipic acid separation. This process consists of the selective aerobic glucose oxidation to glucaric acid and the subsequent hydrodeoxygenation to adipic acid. Stable operation for 1200h TOS with high on-path selectivities of 85-90% was demonstrated for glucose oxidation [2-3].

Hydroxymethylfurfural (HMF), which is readily available from fructose, can be upgraded by consecutive reduction to hexanetriol (HTO) followed by hydrogenolysis to hexanediol (HDO) [4-5]. Steady state yield to BHMF of 90% over 1000 hours TOS have been reported [4-5]. Pyrolyzed Ni/C was found to be competitive to state of art Ni/alumina.

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.

[1] Diamond, G., Hagemeyer, A., Murphy, V., Sokolovskii, V., *Combinatorial Chemistry & High Throughput Screening* 21, 616-630 (2018) (Review).

[2] US 9,776,945, Preparation and separation of di-carboxylic acid-containing mixture. Assigned to Rennovia, Oct. 3, 2017.

[3] US 10,654,027, Shaped porous carbon products. Assigned to Rennovia, May 19, 2020.

[4] https://www.alvacat.com/pdf/CCE-7_Las_Vegas_2023.pdf

[5] US 9,586,920, Process for production of hexanetriol from 5-hydroxymethylfurfural. Assigned to Rennovia, Mar. 7, 2017.

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.

Evaluation of Novel Platinum Photocatalysts for Hydrosilation-Curable Silicones

Melina Michailidis*, Patrick Stulb, John Leman PhD, Peter J. Bonitatibus Jr., PhD

Rensselaer Polytechnic Institute, USA

Abstract:

Hydrosilation, a reaction between silane (Si-H) and vinyl groups, is typically accomplished industrially for release coatings by crosslinking at high temperatures. An environmentally conscious alternative to a heat cure, namely photopolymerization, is actively being explored due to the advantage that it is a low temperature crosslinking process. Catalysts of the type ArCpMePtMe3, where Ar = naphthyl, fluoronaphthyl, and methoxynaphthyl, are hypothesized to accelerate photocatalytic curing due to the installment of ligands containing light-harvesting "antennas". The performance of these catalysts can be assessed relative to industry standard CpMePtMe3 (Pt-99) by monitoring the crosslinking of model silanes via ATR-FTIR. The two vibrational modes of the Si-H bond allow for percent consumption of the hydride to be extrapolated from the decrease in peak area over time, as demonstrated in trial runs with room-temperature catalysts. Eco-inspired innovation of the curing process will produce novel Pt(IV) photocatalysts that can be evaluated against the current benchmark.

Biography:

Melina Michailidis is a first-year graduate student in the accelerated BS/PhD program at Rensselaer Polytechnic Institute (RPI) in Troy, New York. She received a bachelor's degree in chemistry from RPI in May of 2023 and is interested in synthesis, characterization, and evaluation of novel organometallic catalysts.

Molecular Glues vs PROTAC Drugs, Future of Targeted Protein Degradation Therapy

Tauseef Butt

Progenra Inc, Malvern, PA

Abstract Not Available!!!

Catalytic Conversion of CO2 to Syngas Over CeO2 Based Catalysts

Anand Kumar

Qatar University, Qatar

Abstract Not Available!!!

The End

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