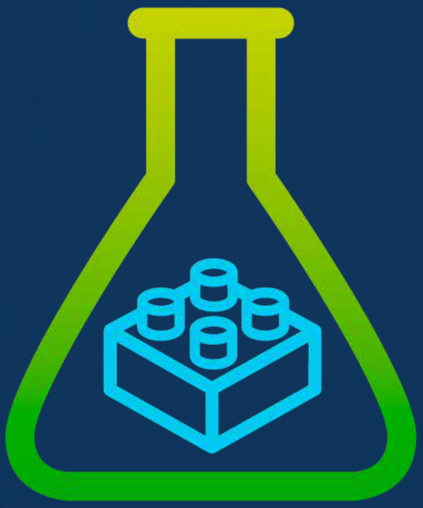
CATALYSIS WEBINAR

BOOK OF ABSTRACTS

SCHOLARS INTERNATIONAL WEBINAR ON

CATALYSIS, CHEMICAL ENGINEERING & TECHNOLOGY

NOVEMBER 25-26, 2021
ONLINE | VIRTUAL



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PROGRAM

Day 1 | November 25, 2021 11:00-18:00 (GMT)

KEYNOTE FORUM

11:00-11:10 GMT Opening Ceremony

11:10-11:40 GMT
Osman Adiguzel, Firat University, Turkey
Title: Thermomechanical and Thermoresponsive Reactions in the Reversibility of Shape Memory Alloys

11:40-12:10 GMT
Irmgard Frank, Leibniz Universität Hannover, Germany
Title: How chemistry leads to deterministic quantum mechanics

12:10-12:40 GMT
Bunsho Ohtani, Institute for Catalysis, Hokkaido University, Japan
Title: Design, Preparation and Characterization of Photofunctional Materials Based on Energy-resolved Distribution of Electron Traps

12:40-13:10 GMT
Joseph Merola, Virginia Polytechnic Institute and State University, USA
Title: Making Effective and Selective Homogenous Catalysts with "Off-the-Shelf" Components

13:10-13:25 - Refreshments Break

KEYNOTE FORUM

13:25-13:55 GMT
Marc Pera-Titus, Cardiff University, UK
Title: Catalysis on Particle-Stabilized Bubbles

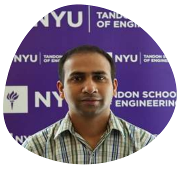
13:55-14:25 GMT
Horia Metiu, University of California, USA
Title: Hydrogen manufacture without CO2

PROGRAM

Day 1 | November 25, 2021 11:00-18:00 (GMT)

SCIENTITIF SESSIONS

14:25-14:45 GMT
Yuri Tulchinsky, Hebrew University of Jerusalem, Israel
Title: Sulfonium Cations as Phosphine Analogs



14:45-15:05 GMT
Ayaskanta Sahu, New York University, Tandon School of Engineering, USA
Title: 2D Transition Metal Dichalcogenide Nanosheets with Single Atom Dopants as Efficient Catalysts for Hydrotreating

15:05-15:25 GMT
Fahri Akalin, ITU/YDO, Turkey
Title: eCAT-COAT TECHNOLOGY Novel Catalytic Applications

15:25-15:45 GMT
Bright Kusema, Solvay, China
Title: Selective hydrogenation of aliphatic amides to amines over heterogeneous catalysts

15:45-16:00 - Refreshments Break

16:00-16:20 GMT
Martin Kotora, Charles University, Czech Republic
Title: Design, Synthesis, and Properties of Indenofluorenes

16:20-16:40 GMT
Geun Ho Gu, KAIST, Republic of Korea
Title: AI Enhanced Computational Catalysis Science

16:40-17:00 GMT
Karina Torres-Rivero, Universitat Politècnica de Catalunya (UPC) - BarcelonaTECH, Spain
Title: Sustainable Silver and Gold Nanoparticles for the Functionalization and Electrocatalytic Enhancement of Screen Printed Electrodes

PROGRAM

Day 1 | November 25, 2021 11:00-18:00 (GMT)

SCIENTITIF SESSIONS

17:00-17:20 GMT
Lohit Sharma, Lehigh University, USA
Title: High selectivity of Sn-modified alumina for propane dehydrogenation under H2S treatment and co-feed

17:20-17:40 GMT
Athule Ngqalakwezi, Advanced Materials Division, Mintek, South Africa
Title: Study of the N-doping effect in graphene nanocomposite for hydrogen storage applications

17:40-18:00 - B2B Meetings and Networking

Day 2 | November 26, 2021 11:00-18:00 (GMT)

KEYNOTE FORUM

11:00-11:10 GMT Opening Ceremony

11:10-11:40 GMT
Annemie Bogaerts, University of Antwerp, Belgium
Title: Plasma technology for electrification of chemical reactions

11:40-12:10 GMT
Maurizio Benaglia, Università degli Studi di Milano, Italy
Title: Flow chemistry, organoatalysis and 3D-printing: Valuable tools in the synthesis of chiral compounds

12:10-12:40 GMT
Nataša Novak Tušar, National Institute of Chemistry and University of Novo Gorica, Slovenia
Title: Engineering photocatalysts for clean air

12:40-13:10 GMT
Jose C Conesa, Instituto de Catálisis y Petroleoquímica, Spain
Title: Sulfide-based photocatalysts using visible light - A review

13:10-13:25 - Refreshments Break

PROGRAM

Day 2 | November 26, 2021 11:00-18:00 (GMT)

13:25-13:55 GMT
Lan Guan, Texas Tech Univeristy Health Sciences Center, USA
Title: Cooperative binding mechanism is the core of co-transport catalyzed by melibiose transporter MelB

13:55-14:25 GMT
Simona Liguori, Clarkson University, USA
Title: Metallic Membranes for Highly Intensified Ammonia Synthesis

SCIENTITIF SESSIONS

14:25-14:45 GMT
Marita Piglowska, Poznan University of Technology, Poland
Title: Carbon-silicon hybrid as anode material in energy sources

14:45-15:05 GMT
Erde Can Safak, Yeditepe University, Turkey
Title: Copolymers of poly(propylene fumarate) with phosphonic acid-based monomers designed as bone tissue engineering scaffolds

15:05-15:25 GMT
Christian Paglia, Supsi imc, Switzerland
Title: Mechanical properties and environmental degradation in high strength aluminum alloys

15:25-15:45 GMT
Pooja Shandilya, Shoolini University, India
Title: Highly efficient dual step-scheme Bi2WO6/Fe2O3/WO3 heterojunction for the photodegradation of bisphenol-A

15:45-16:05 GMT
Jie Gao, University of Oklahoma, USA
Title: Polysaccharide Chemistry and Rheology

16:05-16:20 - Refreshments Break

16:20-16:40 GMT
Xiaoming Miao, Wuxiapptec, China
Title: Kinetic selection in the out-of-equilibrium autocatalytic reaction networks that produce macrocyclic peptides

PROGRAM

Day 2 | November 26, 2021

11:00-18:00 (GMT)

SCIENTITIF SESSIONS

16:40-17:00 GMT
Sara Kawrani, Lebanese American University, Lebanon
Title: Enhancement of photoelectrochemical performance of (CCTO) using different nanosheets, graphene oxide and boron nitride

17:00-17:20 GMT
Cayleigh O'Hare, Illinois Mathematics and Science Academy, USA
Title: Designing a multi-material nerve graft utilizing novel biofabrication techniques to promote peripheral nerve regeneration in injuries greater than 5 cm

17:20-17:40 GMT
Sourav Biswas, State University of New York, USA
Title: Heterogeneous Oxidation Catalysis: A Sustainable Route for Fine Chemical Production

17:40-18:00 GMT
Avinash B Lende, National Tsing Hua University, Taiwan
Title: Hydrogenation of Polyethylene Terephthalate to Environmentally Friendly Polyester by the Heterogenous Catalyst

18:00-18:20 GMT
Sree Pradipta Roy, University of Wisconsin Milwaukee, USA
Title: Asymmetric Reduction of Carbonyl on Clean and Chirally Modified Single Crystal Model Pd and Pt Catalysts

18:20-19:00 - **B2B Meetings and Networking**

CATALYSIS WEBINAR

KEYNOTE PRESENTATIONS
(DAY 01)

SCHOLARS INTERNATIONAL WEBINAR ON

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Title: Thermomechanical and Thermoresponsive Reactions in the Reversibility of Shape Memory Alloys

Osman Adiguzel
Department of Physics, Firat University, Elazig, Turkey

Biography:

Osman Adiguzel graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD- degree from Dicle University, Diyarbakir-Turkey. He studied at Surrey University, Guildford, UK, as a post doctoral research scientist in 1986-1987, and his studies focused on shape memory alloys. He worked as research assistant, 1975-80, at Dicle University and shifted to Firat University in 1980. He became professor in 1996, and he has already been working as professor.

Abstract:

Shape memory effect is a peculiar property exhibited by a series of alloy systems in the β-phase fields, called shape memory alloys. This phenomenon is initiated by thermomechanical treatments, by cooling and deformation; and performed thermally by heating and cooling after thermomechanical processes. These alloys have dual characteristics called thermoelasticity and superelasticity, governed by thermal and mechanical reactions, thermal and stress induced martensitic transformations, and performed thermally and mechanically.

Thermal induced transformation occurs along with lattice twinning on cooling and ordered parent phase structures turn into twinned martensite structures. Twinned martensite structures turn into detwinned martensite structures by means of stress induced transformation by deforming plastically in martensitic condition. Strain energy is stored in the material with deformation and released upon heating, by recovering the original shape in bulk level, and cycles between original and deformed shapes on heating and cooling, respectively.

Superelasticity is also a result of stress induced martensitic transformation and performed mechanically stressing and releasing in the parent austenite phase region. The materials are stressed just over Austenite finish temperature, and shape recovery is performed simultaneously upon releasing the applied stress. The ordered parent phase structures turn into the detwinned structures by means of stress induced martensitic transformation, like the deformation step in shape memory. Superelasticity is performed in non-linear way, unlike normal elastic materials, loading and unloading paths in stress-strain diagram are different, and hysteresis loop reveals energy dissipation.

Shape memory effect is performed thermally in a temperature interval depending on the forward and reverse transformation, on cooling and heating, respectively, and this behavior is called thermoelasticity. Deformation at different temperatures in intermediate region between Martensite start and Austenite finish temperatures exhibits different behavior beyond shape memory effect and superelasticity, and the materials partially recover original shape. Thermal induced martensitic transformation occurs with the cooperative movement of atoms on {110}-type planes of austenite matrix, by means of shear-like mechanism.

Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures. Lattice twinning and lattice invariant shears are not uniform in these alloys, and the ordered parent phase structures martensitically undergo the non-conventional complex layered structures on further cooling.The long-period layered structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice.

In the present contribution, x-ray diffraction and transmission electron microscopy studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns reveal that both alloys exhibit super lattice reflections inherited from parent phase due to the displacive character of martensitic transformation. X-ray diffractograms taken in a long-time interval show that diffraction angles and intensities of diffraction peaks change with the aging time at room temperature. This result reveals a new transformation in displacive manner.

Keynote Speaker
CATALYSIS WEBINAR 2021

Title: How chemistry leads to deterministic quantum mechanics

IRMGARD FRANK
Leibniz Universität Hannover, Germany

Biography:

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

Abstract:

The simulation of chemical reactions is the holy grail of quantum chemistry. In the end one wants to see movies that show the nuclear motion. In addition, it is nice to see the motion of the electronic cloud accompanying and explaining this nuclear motion. Of course, we follow the Rutherford picture of very small nuclei (femtometer scale) within an atom (picometer scale). We lose no accuracy if we describe the nuclei as classical point charges. As it turns out, we have indeed no alternative to this picture, if we describe the electronic cloud with the Schrödinger equation. Consistently, we can move the nuclei with classical Newton dynamics. This approach is already implemented as ab-initio molecular dynamics – unfortunately: we arrive at nothing new, trial and error already led there; fortunately: we can immediately test this approach. It turns out that this deterministic version of quantum mechanics describes reactions, including photo reactions, just perfectly. A vibrational zero-point energy is not needed, the electronic zero-point energy is more than enough. From comparison to experiment at normal energies, we get no hint how to improve this theory of classical nuclear motion. It works fine at normal energies. Classical nuclear motion has philosophical implications: Schrödingers cat dies deterministicly. Note that our approach is not identical with Bohm mechanics. Instead of a guidance equation we simply have Newtons equation.

Title: Design, Preparation and Characterization of Photofunctional Materials Based on Energy-resolved Distribution of Electron Traps

BUNSHO OHTANI
Institute for Catalysis, Hokkaido University, Japan

Biography:

The research work on photocatalysis by Professor Bunsho Ohtani started in 1981 when he was a Ph. D. course student in Kyoto University.Since then he has been studying photocatalysis and related topics for 40 years and published more than 300 original papers (h-index: 70) and two single-author books. After gaining his Ph. D. degree from Kyoto University in 1985, he became an assistant professor in the university. In 1996, he was promoted to an associate professor in Graduate School of Science, Hokkaido University and was then awarded a full professor position in the Catalysis Research Center (presently Institute for Catalysis), Hokkaido University in 1998. He was awarded several times form the societies related to chemistry, photochemistry, electrochemistry and catalysis chemistry.

Abstract:

How can we design solid photocatalysts? What is the decisive factor controlling photocatalytic activities? So-called band-structure model (BSM), electrons in a valence band (VB) of a photocatalyst is photoexcited to a conduction band (CB), leaving positive holes in VB, and electrons and holes reduce and oxidize, respectively, substrates adsorbed on the surface of the photocatalyst, does suggest preferable band positions for redox reaction uniquely decided only by crystalline structure. The other possible factors, e.g., particle size and surface structure, cannot be discussed within BSM. Recently, we have developed reversed double-beam photoacoustic spectroscopy (RDB-PAS) which enables measure energy-resolved density of electron traps (ERDT). Those electron traps (ETs) seem to be predominantly located on the surface of almost all the metal oxide particles, with exception of nickel oxide and therefore they reflect macroscopic surface structure in ERDT patterns. Using ERDT pattern with the data of CB-bottom position (CBB), i.e., ERDT/CBB patterns, it has been shown that metal oxide powders can be identified without using the other analytical data such as X-ray diffraction patterns or specific surface area, and similarity/differentness of a pair of metal-oxide samples can be quantitatively evaluated as degree of coincidence of ERDT/CBB patterns. In this talk, a novel approach of material design based on the ERDT/CBB patterns is introduced.

Keynote Speaker
CATALYSIS WEBINAR 2021

CATALYSIS WEBINAR

Title: Making Effective and Selective Homogenous Catalysts with “Off-the-Shelf” Components

JOSEPH MEROLA
Virginia Tech, United States

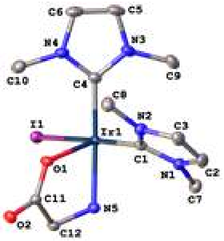
Biography:

Joseph S. Merola is a Professor of Chemistry at Virginia Tech and a graduate of Carnegie-Mellon University (B.S. Chemistry, 1974). He received his Ph.D. in chemistry in 1978 from M.I.T under the direction of Professor Dietmar Seyferth. In 1978, he joined the Corporate Research Laboratories of Exxon Research and Engineering Co in New Jersey. In 1987, he joined Virginia Tech where he has been ever since, although he has held many different roles over his time there. Professor Merola is a Fellow of the American Chemical Society and a Fellow of the American Association for the Advancement of Science. He has published over 120 papers in the organometallic chemistry and catalysis field.

Abstract:

A series of chiral complexes of the form Ir(NHC)2(aa)(H)(X) (NHC =N-heterocyclic1carbene, aa = chelated amino acid, X = halide) was synthesized by oxidative addition ofα-amino2acids to iridium(I) bis-NHC compounds and screened for asymmetric transfer hydrogenation of3ketones. Following optimization of the reaction conditions, NHC, and amino acid ligands, high4enantioselectivity was achieved when employing the Ir(IMe)2(L-Pro)(H)(I) catalyst (IMe = 1,3-5dimethylimidazol-2-ylidene), which asymmetrically reduces a range of acetophenone derivatives6in up to 95% enantiomeric excess.

This approach yields excellent homogenous catalysts without the need to carry out specialized or intricate ligand design since all components (NHCs, amino acids) are either relatively inexpensive, commercially available products or very easily synthesized.



Title: Catalysis on Particle-Stabilized Bubbles

MARC PERA-TITUS
Cardiff University, UK

Biography:

Marc Pera-Titus is Professor & Chair of Sustainable Catalytic Chemistry at Cardiff University (Wales, UK). Marc received a double MSc degree in Chemical Engineering (2001) and Physical Chemistry (2002), and a PhD (2006) from University of Barcelona (Catalonia, Spain). In 2007, he joined Ircelyon/CNRS (France) as postdoc and was further appointed CNRS fellow in 2008. From 2011-2020, Marc was project leader, expert and deputy director at the E2P2L CNRS-Solvay joint laboratory in Shanghai (China), merging industrial and academic research. Marc is author of 125 papers and inventor of 16 patents in the fields of membranes, adsorption, catalysis and process eco-design. Marc has received numerous awards, including the Rhone-Alpes Foundation Award (2007), the Elsevier Award for highly cited author in Catalysis (2009), the Silver and Gold Medals from the Chinese Academy of Inventions (2016, 2017), the DivCat award from the French Society of Chemistry (2017) and a ERC consolidator grant (2018). Since 2021, he is elected fellow of the Royal Society of Chemistry.

Abstract:

Gas-liquid-solid (G/L/S) reactions are ubiquitous in chemical, petrochemical and environmental catalytic processes. Conventional G/L/S reactors comprise packed beds, stirred tanks and bubble column slurry reactors. These technologies usually suffer from mass/heat transfer limitations due to low G/L and L/S specific interface areas and poor gas solubility. As a way out, herein we developed particle-stabilized foams and bubbles in water and organic solvents as efficient G/L/S microreactors for conducting diffusion-free catalytic reactions at low gas pressures.

First, we prepared oil foams stabilized by surface-active silica particles bearing fluorinated chains and Pd nanoparticles. Foamability increased with both the particle concentration and stirring rate. High foam stability was achieved in benzyl alcohol / xylene mixtures at very low particle concentration (<1 wt%) for contact angles in the range 41-73°. The catalytic performance was strongly affected by the foaming properties, with 8-times activity increase in pure O2 compared to non-foam systems. Particles were conveniently recycled with high foamability and catalytic efficiency maintained for at least 7 consecutive runs. Besides xylene, other solvents with surface tension lower than that of the substrate could tune the particle wettability, enhancing the foamability and catalytic performance in the aerobic oxidation reactions of a panel of alcohols.

In a next step, we engineered an on-purpose microfluidic tool to generate and test monodisperse bubbles in solvents stabilized by fluorinated silica particles (Figure 1). Bubble trapping and particle adsorption/desorption dynamics was studied using fluorescent particles adsorbed at the air/oil interface. Accumulation of particles at the back of bubbles was observed. When the confined bubbles left to the wider channel, the interface relaxed and became circular with redistribution of adsorbed particles. We compared the catalytic performance of particle-stabilized bubbles using amphiphilic catalysts able to adsorb at the G/L interface in model oxidation reactions, showing promising credentials compared to stirred tank G/L/S reactors.

Keynote Speaker
CATALYSIS WEBINAR 2021

Title: Catalysis on Particle-Stabilized Bubbles

MARC PERA-TITUS
Cardiff University, UK

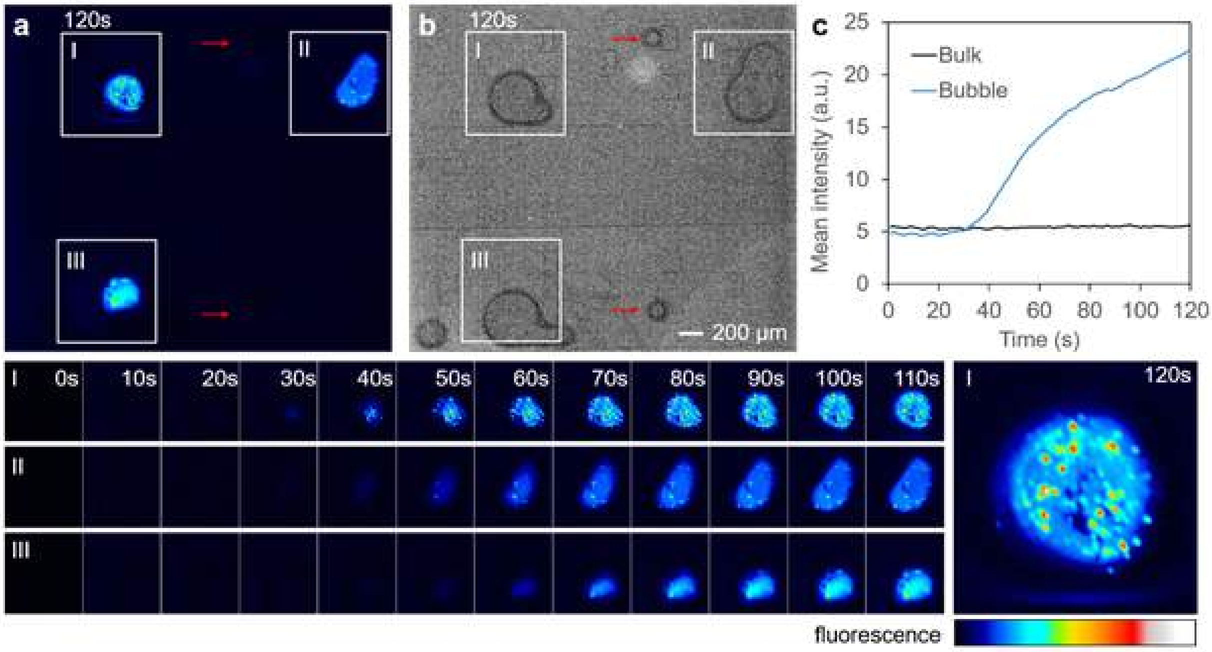


Figure 1. Catalysis on a particle-stabilized bubble. a) Fluorescence images of the microfluidic chip after 2 min, where (I-III) indicate the time-lapse of corresponding chip regions; b) Same as (a) but in gray scale representation and with busted image brightness to show all bubbles present in the chip (stable monodisperse bubbles indicated with the arrows produce no fluorescent signal); c) Time-evolution of the mean fluorescence intensity across the bubble (region I) and in the bulk. Conditions: outer phase (Qs = 150µL/minm, 1 mM H2DCF-DA in DMSO); middle phase (Qp = 150µL/min, 4 wt% Pd@F-particles in octanol with 10 mM t-BuOK; air pressure P = 400 mbar; temperature 80 °C.

Title: Hydrogen manufacture without CO2

HORIA METIU
University of California, USA

Biography:

Horia Metiu obtained his Ph.D. at MIT in 1974. After postdoctoral research at MIT and the University of Chicago, he joined the UCSB faculty in 1976. His awards include the Exxon Solid State Chemistry ACS award (1979), the UCSB Faculty Research Lectureship (1987), a Humboldt Senior Scientist Award (2003), and the American Chemical Society Division of Physical Chemistry Award in Theoretical Chemistry (2015). He was an Associate Editor of the Journal of Chemical Physics from 1999 through 2012. His current research focus, in collaboration with experimentalist colleagues, is on the search for new catalysts for converting natural gas or CO_2 into useful chemicals.

Abstract:

Most hydrogen is currently produced by steam reforming of methane or other hydrocarbon feedstock. The manufacture of roughly 50 million tons of H_2 produces 300 million tons of CO_2 as a side product. Catalytic methane pyrolysis, $CH_4 = C + 2H_2$ is a possible alternative. Performing this reaction without a catalyst requires unreasonably high temperature.The use of traditional catalysts is not possible because of coking. To avoid coking we began a systematic search for molten catalysts. The reaction is performed in a bubble column in which methane is injected in the molten catalyst. The reaction takes place in the bubbles and the carbon form is carried with the bubble and it floats on top of the melt from which it can be removed.In this implementation the catalyst in the liquid carbon remains clean and there is no coking. We have studied both molten metal alloy catalysts and molten salts. I will present results for the best-performing catalysts we have found.We have also studied dry methane reforming catalyzed by molten metals. Pyrolysis and dry reforming occur concurrently and this allows the production of syngas of any desired ratio of hydrogen to CO. As in the case of pyrolysis there is no coking.

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SCIENTIFIC SESSIONS
(DAY 01)

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Title: Reviving the Coordination Chemistry of Sulfonium Cations

Yuri Tulchinsky
Hebrew University of Jerusalem, Israel

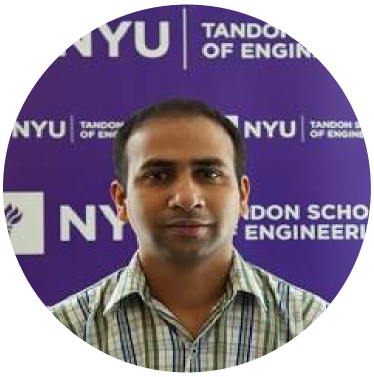
Biography:

Dr. Yuri Tulchinsky has competed his PhD at the Technion – Israeli Institute of Technology in the field of organometallic chemistry with Prof. M. Gandelman in 2014. He then joined the group of Prof. M. Dinca at MIT where he worked on metal organic frameworks (MOF). Since 2018 Dr. Tulchinsky has been appointed as an Assisting Professor at the Hebrew University of Jerusalem. His research interests span different areas of organic, organometallic and supramolecular chemistry, in particular, development of unusual ligand frameworks for future applications in homogeneous catalysis.

Abstract:

Sulfonium ions are more than a century old and have countless applications in organic synthesis and homogeneous catalysis. However, unlike the isoelectronic tertiary phosphines, which became nearly indispensable in homogeneous catalysis, the potential of sulfonium ions to act as ancillary ligands remained unexplored for decades since the first few structures were reported.

In this talk I will describe the synthesis and full characterization of the first Rh(I) and Pt(II) complexes of sulfonium ligands, thus showing that the very limited pool of known sulfonium complexes can be extended to metals widely used in catalysis. Moreover, for the first time, the coordinating ability of an aromatic sulfonium cation has been established. I will also present a comprehensive computational study of these complexes which not only attests for the π-accepting nature of sulfonium cations, but also places them among the most π-acidic ligands available. This work strongly suggests the perspective of sulfonium ions becoming key players in π-acid catalysis.



Title: 2D Transition Metal Dichalcogenide Nanosheets with Single Atom Dopants as Efficient Catalysts for Hydrotreating

Ayaskanta Sahu
New York University, USA

Biography:

Ayaskanta Sahu is an Assistant Professor in the Department of Chemical and Biomolecular Engineering at the New York University Tandon School of Engineering. His research focuses broadly on how to develop artificial materials that do not exist in nature; how to derive novel properties from existing materials by tuning their size (nanostructuring) and adding trace amounts of intentional impurities (doping); and finally how to incorporate these materials into functional devices that can harness new forms of energy or improve the efficiency of existing energy conversion devices. Prior to joining NYU, he was a Materials Postdoctoral Fellow at the Molecular Foundry, Lawrence Berkeley National Laboratory in Berkeley, California. He holds a B. Tech. degree in Chemical Engineering from the Indian Institute of Technology Roorkee and a Ph.D. in Chemical Engineering from the University of Minnesota. He spent a couple of years at ETH Zurich as a visiting scientist before joining LBNL.

Abstract:

Tailoring highly efficient catalysts is of utmost importance to reduce the carbon and energy footprints of industrial processes. An important class of industrial chemistries is hydrotreating whereby heteroatoms such as sulfur, oxygen, and nitrogen in carbon-containing feedstocks (hydrocarbons and biomass) are removed catalytically using molecular hydrogen. Transition metal dichalcogenides, such as molybdenum sulfide (MoS2), have been employed in bulk form commercially as hydrodesulfurization catalysts due to their widespread availability. In the nanoscale, MoS2 forms stable two-dimensional nanosheets, which exhibit impressive catalytic activity along the nanosheet edge sites. Conversely, the non-edge atoms of the basal plane are sufficiently coordinated and thus relatively inert. Given that a large portion of the surface area is inactive, there is a strong impetus towards modifying and nanostructuring 2D materials to activate the basal plane, such as through decorating the surface with singular dopant atoms to create isolated single-atom active sites that may possess novel catalytic properties for hydrogenation/hydrogenolysis chemistries. Here, we demonstrate the controlled, tunable in-situ cobalt doping of MoS2 nanosheets grown via colloidal hot-injection method. A set of catalysts with various cobalt loadings were studied for hydrodesulfurization of thiophene and hydrodeoxygenation, specifically probing the effects of dopant concentration and local structure of single cobalt atoms, inferred from x-ray absorption spectroscopy and density functional theory (DFT), on catalytic activity. We demonstrate that the relationship between dopant concentration and thiophene conversion is non-linear, and an optimal cobalt loading exists for these hydrotreating reactions.

Title: eCAT-COAT TECHNOLOGY Novel Catalytic Applications

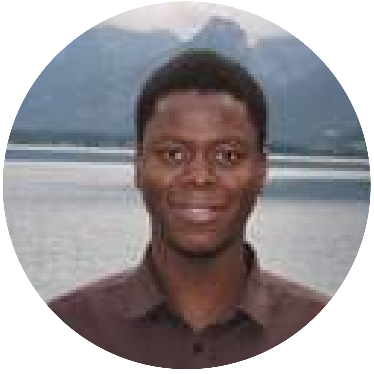
FAHRI AKALIN
ITU/YDO, BSc in Marine Engineering Dept, Turkey

Biography:

I was born on April, 1st 1949 in Aydin/Turkey, graduated ITU/YDO, BSc in Department of Marine Engineering on 1970 at Istanbul/Turkey. Now I am Retired at Home from SSK since Mar 1992 - Present.

Abstract:

The technology is emitted into its environment and utilized by itself other form of energy other than existence known energy forms. The energy itself is assumed to have a minute wavelength and can therefore not be measured by instruments currently available to science, but also the results derived from its practical application can be measured, quantified and replicated The technology based on hydrogen bond catalysis is a type of organosilicon catalysis that relies on use of hydrogen bonding interactions to accelerate and control naturally organic reactions. In biological systems, hydrogen bonding plays a key role in many enzimatic reactions both in orienting the subsrate molecules and lowering barriers to reaction. Result in to perform catalytic applications using the power of hydrogen bonds.The products are energy printed carrier materials and applicable to our everyday activity process ranging from practical, industrial, agricultural and environmental problems can be solved. The reactions produced by the technology application breaks the hydrogen bonds or removes the hydrogen bar. The cluster in this way is kept smaller (nano clustered water and /or liquid /fluid), and the water and /or liquid /fluid characteristics return to the original water and/or fluid/liquid form. These reactions scientifically well known as stabilisation -homogenisation.



Title: Selective hydrogenation of aliphatic amides to amines over heterogeneous catalysts

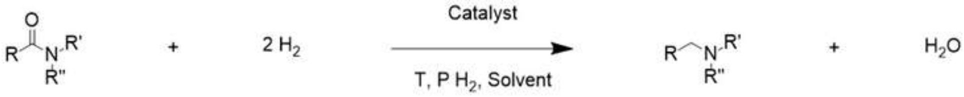
Bright Kusema
Solvay, China

Biography:

Dr. Bright T. Kusema studied and received his M.Sc. degree in Chemical Engineering and Biotechnology at the D. I. Mendeleev University of Chemical Technology of Russia (2007). He obtained his Ph.D. degree in Chemical Engineering, within the field of industrial chemistry and reaction engineering at Åbo Akademi University in Finland (2011). He was a postdoctoral researcher at Åbo Akademi University, Finland and ETH Zürich, Switzerland in advanced catalysis engineering. He has been working in the industry as a Research Scientist in eco-efficient products and processes at Solvay. In 2020, he was awarded the title of Docent in Industrial Catalysis.

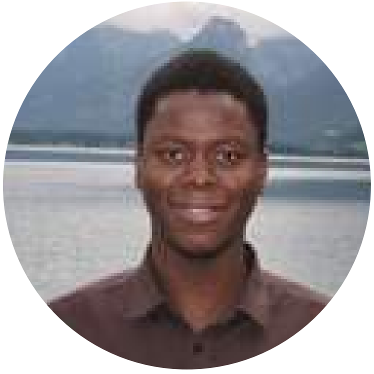
Abstract:

The selective catalytic reduction of amides using molecular hydrogen is an attractive synthesis route for the green and sustainable production of amines at industrial scale. The hydrogenation reaction is an atom efficient and environmentally benign process as water is the only by-product generated. In addition, the heterogeneous catalyst can be recycled and reused. The resulting amines are widely used in the industry for the production of pharmaceuticals, agrochemicals, surfactants, dyes and polymers. In this work, a highly efficient catalytic hydrogenation system was developed for the selective transformation of aliphatic amides to the corresponding amines at relatively mild reaction conditions (Scheme 1).



Scheme 1. Selective hydrogenation of aliphatic amides to amines over heterogeneous catalyst.

Industrial hydrogenation catalysts such as Pd/Al2O3, Pt/Al2O3 and Rh/Al2O3 were modified with vanadium (V) or molybdenum (Mo) species as oxophilic centers. The modified catalysts were prepared by deposition of V or Mo precursor on supported catalysts via impregnation method. The catalysts were characterized by several techniques, such as, ICP-OES, XRD, XPS, H2-TPR, FTIR, CO-chemisorption, TEM, SEM-EDX and TGA. Modified Rh-V/Al2O3 catalyst displayed the best performance affording high yield and selectivity > 95 % to the desired tertiary and secondary amines at moderate reaction conditions of T < 130 °C and P H2 < 50 bar (Figure 1).



Title: Selective hydrogenation of aliphatic amides to amines over heterogeneous catalysts

Bright Kusema,
Solvay, China

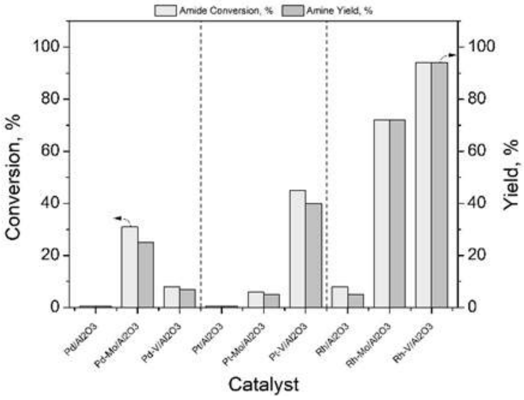


Figure 1. Catalyst screening in hydrogenation of aliphatic amide to amine.

The strong synergistic interaction and proximity of hydrogenation Rh0 sites and oxophilic Vδ+ sites in the bimetallic Rh-V/Al2O3 catalyst were determined to be beneficial for the selective dissociation of C=O bond of the carboxamides into the desired amines.

Title: Design, Synthesis, and Properties of Indenofluorenes

Martin Kotora
Charles University, Czech Republic

Biography:

Martin Kotora obtained a MsC degree in 1986 from Charles University in Prague a PhD degree in 1991°from the Institute of Chemical Process Fundamentals, the Czech Academy of Sciences. He became a postdoc at the Institute for Molecular Science in Okazaki and later at Purdue University. In 1996 he joined the faculty at the Catalysis Research Center, Hokkaido University. In 2000 he returned to his alma mater (Charles University) where he has been ever since as a full professor. His group's research interests center around transition metal complex catalyzed or mediated reactions and their application in organic synthesis.

Abstract:

Aromatic compounds are fascinating class of substances that have attracted attention of the whole chemical community for since early days of modern chemistry. In this respect, substances possessing the fluorene or indenofluorene scaffolds constitute a class of compounds that might find in organic material sciences. Therefore, development of new and general synthetic procedures is of general interest. Among numerous synthetic strategies leading to this class compounds, the one based on catalytic cyclotrimerization of suitably substituted and easy to prepare alkyne precursors offers a number of advantages. However, this approach has not been extensively studied, despite of some promising results in the field of fluorene synthesis,

The potential of catalytic alkyne cyclotrimerization was initially applied in successful synthesis of various unsymmetrically substituted fluorenes. As far as transition-metal based catalytic systems were concerned, those based on Rh-complexes provide the best results in the term of conversion and also structural variability in the starting material. The results prompted further extension of this methodology to synthesis of selectively substituted [5]- and [7]helical indenofluorenes and their substituted derivatives. Gratifyingly, the use chiral Rh-complexes allowed to carry out the cyclotrimerization enantioselectively forming [7]helical indenofluorenes with high asymmetric induction (up to 95% ee). As far as physical properties of fluorenes and indenofluorenes are concerned, they are highly fluorescent emitters in the range of UV and blue light region. The emission wavelength can be controlled by suitable substitution of the basic scaffold and degree of -conjugated systems. Chiral [7]helical indenofluorenes are CPL active compounds with glum = ~10-3. In addition, upon deposition on Au surface undergo [7]helical indenofluorenes planarization forming unusual polyaromatic hydrocarbons.

Title: AI Enhanced Computational Catalysis Science

Geun Ho Gu
KAIST, Republic of Korea

Biography:

Geun Ho's research focuses on data-driven machine-learning methods, and multiscale modeling strategies to understand complex chemistry and catalysis phenomena and to establish high-throughput materials design methods. He obtained his B.S. in chemical and biomolecular engineering at the University of Illinois at Urbana-Champaign (2012), and his Ph.D. in chemical engineering at the University of Delaware (2018) in the Vlachos research group. Geun Ho is currently a post-doctorate researcher at the KAIST advised by Professor Yousung Jung, looking for a faculty position.

Abstract:

Aromatic compounds are fascinating class of substances that have attracted attention of the whole chemical community for since early days of modern chemistry. In this respect, substances possessing the fluorene or indenofluorene scaffolds constitute a class of compounds that might find in organic material sciences. Therefore, development of new and general synthetic procedures is of general interest. Among numerous synthetic strategies leading to this class compounds, the one based on catalytic cyclotrimerization of suitably substituted and easy to prepare alkyne precursors offers a number of advantages. However, this approach has not been extensively studied, despite of some promising results in the field of fluorene synthesis,

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Title: Sustainable Silver and Gold Nanoparticles for the Functionalization and Electrocatalytic Enhancement of Screen Printed Electrodes

Karina Torres-Rivero
Universitat Politècnica de Catalunya (UPC) - BarcelonaTECH, Spain

Biography:

Karina Torres-Rivero; currently, I am a Ph.D. student and researcher at the Universitat Politècnica de Catalunya in Barcelona, Spain. I am working with the Resource Recovery and Environmental Management (R2EM) investigation group. We are focused on developing new sensors with nanoparticle surface modifications to determine heavy metal contaminants in water. Also, we are studying the nano and microparticles utilization to remediate contaminated soils. My ultimate goal is the possibility to use the modified electrodes for heavy metal determination in acid mine drainage and extract all the available heavy metal content to synthesize chemical and green nanoparticles within the circular economy action plan.

Abstract:

Screen-printed electrodes (SPEs) functionalization can enhance the electrochemical response towards specific analytes. Usually, synthesized metal nanoparticles (MNPs) employing physical and chemical strategies are used to modify SPEs but, recent developments have shown the utilization of biological reactants such as leaf, flowers, and fruits extracts in the production of MNPs. Thus, green silver (G-AgNPs) and gold nanoparticles (G-AuNPs) were synthesized employing grape stalk waste extract as a reusable organic residue from the wine industry to modify commercial screen-printed carbon nanofiber electrodes (SPCNFEs) for the determination of Pb2+. The G-AgNPs and G-AuNPs were characterized using scanning and transmission electron microscopy (STEM) and nanoparticle tracking analysis (NTA). The G-AgNPs and G-AuNPs were deposited onto SPCNFEs surface using spin coating technique. Also, the modified sensors G-AgNPs-SPCNFE and G-AuNPs-SPCNFE were electrochemically characterized using differential pulse anodic stripping voltammetry (DPASV) towards the determination of Pb+2 in aqueous samples using acetic acid/acetate buffer pH 4.5. The electrochemical characterization allowed the Pb2+ determination with detection limits (LODs) as low as 6.9 µg.L-1 and 6.3 µg.L-1 using G-AgNPs-SPCNFE and G-AuNPs-SPCNFE respectively. These values are even lower than the concentration limit value established by the drinking water European legislation, 10 µg.L- 1, making the green synthesized silver and gold nanoparticles modified electrodes a promising alternative to those sensors modified with MNPs obtained by the conventional synthesis methods..

Featured Speaker
CATALYSIS WEBINAR 2021

Title: Sustainable Silver and Gold Nanoparticles for the Functionalization and Electrocatalytic Enhancement of Screen Printed Electrodes

Karina Torres-Rivero
Universitat Politècnica de Catalunya (UPC) -
BarcelonaTECH, Spain

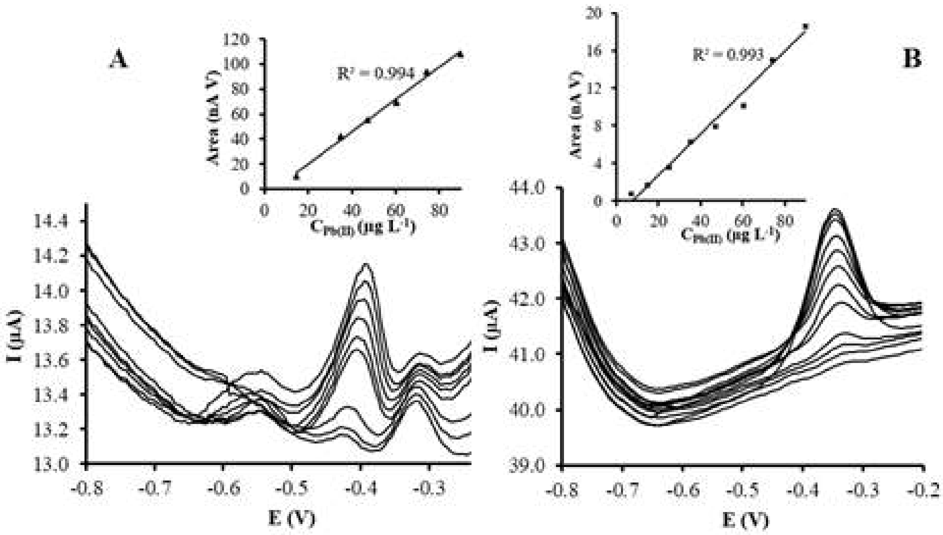

Figure 1. Voltammograms and calibration curve for Pb2+ determination using (A) green-AgNPs-SCPNFEs and (B) green-AuNPs-SPCNFE in acetic acid/acetate pH 4.5, deposition potential (Ed) - 1.2 V, deposition time (td) 180 seconds. DPASV parameters: step potential of 5 mV, pulse time of 50 ms, and pulse amplitude of 50 mV.

Title: High selectivity of Sn-modified alumina for propane dehydrogenation under H2S treatment and co-feed

Lohit Sharma
Lehigh University, USA

Biography:

Currently, Lohit is working as Technology development engineer at Intel Corp. Lohit graduated with a Ph.D. in Chemical Engineering at Lehigh University under the supervision of Prof. Jonas Baltrusaitis and Prof. Israel E. Wachs. Lohit research involves elucidating the reaction kinetics and catalyst structure in the presence of H2S. His research interests include the catalytic conversion of CO2 into chemicals and the catalytic conversion of light alkane through heterogeneous catalysis.

Abstract:

A large share of natural gas reserves is sour and can contain a significant amount of H2S. These streams are typically treated using energy-intensive separation methods to remove sour gas molecules to preserve downstream catalysts and equipment. In contrast, we investigate sour gas tolerant catalysts to devise catalytic processes for sour natural gas monetization without prior CO2 and H2S removal.

The catalytic dehydrogenation of propane (PDH) is the most direct and selective way to produce propylene and valorize propane from abundant natural and shale gas resources. Recent experimental and computation work has demonstrated that earth-abundant and environmentally benign bulk metal oxide, such as Al2O3, TiO2, and ZrO2 can exhibit good activity and selectivity for PDH. Recently, we showed that bulk γ-Al2O3 catalyst shows high selectivity for propane dehydrogenation upon pretreatment and co-feeding with H2S. Subsequently, to improve catalyst selectivity, we have modified alumina by the introduction of Sn to reduce cracking reaction over alumina catalyst. The selectivity is further enhanced from ~94% over Al2O3-S to 98% on 1.5-10 Sn/Al2O3-S at identical operating conditions although a decrease in rate was observed with Sn loading during the first few dehydrogenation cycles. At low loadings, Sn is atomically dispersed and selectively binds to hydroxyl groups or oxygen atoms on Al2O3. This prevents the formation of original (unmodified) defect sites on Al2O3 and improves overall selectivity. The activity and selectivity of the catalyst are heavily dependent on the chemical potential of sulfur and hydrogen because they influence both the relative concentration of the two types of sites and the overall reaction mechanism. Finally, the catalyst can be regenerated fully under a pure H2S stream, thereby precluding treatment under oxygen which can lead to sintering. This study shows that Sn modified alumina as (i) highly selective, (ii) regenerable, (iii) environmentally benign, and (iv) low-cost sulfur tolerant catalysts for large-scale non-oxidative dehydrogenation of propane to propene (PDH) for sour gas up-gradation.

Title: Study of the N-doping effect in graphene nanocomposite for hydrogen storage applications

Athule Ngqalakwezi
Advanced Materials Division, Mintek, South Africa

Biography:

Athule Ngqalakwezi is research scientist at Mintek's advanced materials division in the catalysis division. She completed her Masters at South Africans prestigious university, University of the Witwatersrand and currently in plans to continue to do her PhD.

Abstract:

Graphene, a carbon allotrope, embodies key advancement in modern science through its versatile properties and as such has been considered for many applications such as catalysis, hydrogen storage and sensors. In this work, precursor graphene was synthesized using Improved Tours method and modified hummer's method and later reduced with ammonia and L-Ascorbic acid. Reduced graphene was then incorporated with Ca and Ni to study the effect of N-doping effect on hydrogen storage capacity. The graphene nanocomposite was charged with hydrogen at a pressure of about 10 bars and ambient temperature. Transmission electron microscopy (TEM) was utilized to determine and study the surface morphology of the reduced graphene, graphite oxide and graphene nanocomposite. Elemental analysis of the material was carried out using FTIR and Raman while the phase was determined using powder X-ray diffraction (XRD). The reaction mechanism of the hydrogen uptake on the graphene nanocomposite was investigated. The metal-graphene exhibited acceptable hydrogen uptake. The FTIR and Raman band showed L-Ascorbic reduced the GO better than ammonia through the observed decrease on the functional bands after reduction. The elemental analysis carried out using XRF showed the successful loading of Ca on the graphene matrix. The hydrogen storage capacity of the nanocomposite was tested using TPD equipped with Mass Spectrometer. The Ca/graphene nanocomposite reduced by ammonia exhibited a large hydrogen storage uptake at 4.98 wt. % compared to L-Ascorbic acid.

CATALYSIS WEBINAR

KEYNOTE PRESENTATIONS
(DAY 02)

SCHOLARS INTERNATIONAL WEBINAR ON

CATALYSIS, CHEMICAL ENGINEERING & TECHNOLOGY

NOVEMBER 25-26, 2021
ONLINE | VIRTUAL

https://scholarsconferences.com/catalysis-webinar/

Title: Plasma technology for electrification of chemical reactions

ANNEMIE BOGAERTS
Università degli Studi di Milano, Italy

Biography:
Annemie Bogaerts obtained her PhD diplomas at University of Antwerp in 1996, and is professor since 2003, and full professor since 2012. She is leading the research group PLASMANT, which she started "from scratch", and which currently counts almost 50 members. Her research focuses on plasma chemistry, plasma reactor design and plasma-surface interactions, by experiments and modeling, mostly for green chemistry (plasma catalysis) and medical applications (cancer treatment).
She has above 500 peer-reviewed publications since 1995, and above 18,000 citations, with a H-index of 68 (Web of Science) (above 26,000 citations and H-index of 80 in Google Scholar). She has above 230 invited lectures at international conferences or universities (since 1995). She was the supervisor of 44 finished PhD theses (since 2005), and is now supervising 30 PhD students (incl. several joint PhD students), and 15 postdocs. In 2019, she obtained the prestigious ERC Synergy Grant, the highest recognition in Europe.

Abstract:
Plasma technology is gaining increasing interest for various gas conversion applications, such as CO2 and CH4 conversion into value-added compounds, and N2 fixation for fertilizer applications, i.e., more in general: green chemistry. Plasma is a (partially) ionized gas, created by applying electricity. It consists of electrons, various ions, radicals, excited species, besides neutral gas molecules. The electrons are mainly heated by the applied electric field, due to their small mass, and they activate the gas molecules by electron impact ionization, excitation and dissociation, creating new ions, excited species and radicals. These are very reactive, so they can easily produce new products. Hence, thermodynamically or kinetically limited reactions can proceed at mild conditions of gas temperature and pressure, because the gas activation is accomplished by the electrons. Typically, plasma reactors operate at atmospheric pressure and the gas is introduced at room temperature. Plasma technology has low CAPEX costs. Finally, the plasma reactors can quickly be switched on/off, and because they operate with electricity, they are very suitable to be combined with (fluctuating) renewable electricity, for electrification of chemical reactions. To improve this application in terms of conversion, energy efficiency and product formation, a good insight in the underlying mechanisms is desirable. We try to obtain this by computer modelling, supported by experiments.
I will first give a brief explanation about different types of plasma reactors used for green chemistry applications. That will be followed by an overview of the state of the art in plasma-based CO2 and CH4 conversion, as well as N2 fixation, with these different types of plasma reactors, and a brief discussion of the opportunities and main challenges. Subsequently, I will present some recent results obtained in Antwerp in this domain, including experiments and modeling for a better understanding of the underlying mechanisms.

Keynote Speaker
CATALYSIS WEBINAR 2021

Title: Flow chemistry, organoatalysis and 3D-printing: Valuable tools in the synthesis of chiral compounds

MAURIZIO BENAGLIA
Università degli Studi di Milano, Italy

Biography:

Maurizio Benaglia is Full Professor of Organic Chemistry at the Università degli Studi di Milano, Italy. He is currently Director of ISPROCHEM, International School of Process Chemistry and member of the Scientific Committee of IASOC (Int Advanced School of Organic Synthesis). Author of more than 210 papers, his research interests deal with the development of innovative synthetic methodologies, new chiral catalysts, synthesis of pharmaceutically active compounds, taking advantage of enabling technologies (flow chemistry, microwave, alternative solvents).

Abstract:

Recently developed organocatalytic stereoselective transformations using polymer-based packed bed and catalytic reactors will be presented. Furthermore, the use of different bifunctional chiral metal-free catalysts in micro- and mesofluidic devices will be described. The potential of this flow chemistry approach was demonstrated by the successful synthesis of an advanced intermediate for the preparation of the GABAB receptor agonist Baclofen and other Active Pharmaceutical Ingredients (APIs) such as (S)-Pregabalin and (S)-Warfarin.

Additionally, considering that now 3D-printing technology allows chemists to build devices with high precision and well-defined architecture, an in-house designed, 3D-printed reactors were realised and used for the catalytic synthesis of biologically active compounds.

A recently published continuous flow approach to access -trifluoromethylthiolated esters and amides using commercially available arylacetic acids and N-(trifluoromethylthio)phthalimide as the electrophilic reagent will be also described.

Title: Engineering photocatalysts for clean air

Nataša Novak Tušar
National Institute of Chemistry and University of Novo Gorica, Slovenia

Biography:

Prof. Dr. Nataša Novak Tušar has been the head of the Laboratory of Environmental Science and Engineering 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 at University of Ljubljana, 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).

Abstract:

In today’s world, clean air is one of the top priorities of humanity due to human health and climate change. Air pollution refers to the release of pollutants into the air from industrial processes, transportation, and consumer products. Both controlling the sources of pollution and air cleaning are important for improving air quality. The lecture focuses on the engineering of low-cost and environmentally friendly photocatalysts for indoor air cleaning. Titanium dioxide (TiO2) is the most used material for mentioned application due to its interesting characteristics: low cost, high stability, shows high photocatalytic activity, it can promote ambient temperature oxidation of the major class of organic pollutants. However, due to the hindered applications of TiO2 as non-supported systems for photocatalytic air cleaning, design and development of TiO2 supported systems are very important. Common support materials are SiO2, Al2O3, zeolites (aluminosilicates), carbon etc. These materials exhibit high specific surface areas, high porosities in a variety of pore sizes, and high thermal and mechanical stability, while they are mostly chemically inert. Here, an overview of the design and development of mechanically stable TiO2-SiO2 coatings for removal of the volatile organic pollutants from the air is presented. Engineering of photocatalysts consisting of a) SiO2 supported TiO2 working under UV light and b) SiO2 supported TiO2 functionalized with transition metals working under visible light is discussed.

Title: Sulfide-based photocatalysts using visible light – A review

JOSE C CONESA
Instituto de Catálisis y Petroleoquímica, CSIC, Spain

Biography:
J.C. Conesa entered the permanent research staff of Instituto de Catálisis y Petroleoquímica (ICP) in 1979, becoming there Research Professor in 2004. He was ICP Vicedirector from 2010 to 2014, and Director from 2014 to 2018. He is now Ad Honorem Professor.
He was first in Spain using synchrotron radiation to study heterogeneous catalysis; in CSIC using quantum calculations to study them, and in ICP using microemulsions to make oxide nanoparticles. He works in XPS and FTIR (including operando mode) and in EPR and UV-Vis-NIR spectroscopies. He has worked on metal-support interactions, and on CeO_2-supported metals/oxides. He uses now CeO_2-based combinations for H_2 technologies. He kept always interest in photocatalysis and photoactive solids.
He belongs since 2014 to the Steering Committee of AMPEA. According to the Web of Science database, his over 200 articles and book chapters received to date more than 9700 citations, leading to a Hirsch index h=56.

Abstract:
Sulphides are used frequently for photocatalysis, since they are better absorbers of visible light than oxides; indeed, in some cases they can absorb light even in the near-infrared range. Their drawback is however that they are prone to photocorrosion, mainly in oxidizing conditions; they are therefore more frequently used in reductive processes, e.g. H_2 production or CO_2 reduction to a number of fuels. Here an overview will be given of different sulphides (HgS, Cu_2S, CdS, chalcopyrites, FeS_2, MoS_2, PbS, etc.) used for different photocatalytic processes, giving details of their structures and photocatalytic action and, where appropriate, recent reviews on their behaviour. Results obtained in recent years by our group with several powder sulphides (in particular, In_2S_3, $ZnIn_2S_4$ and SnS_2) will be described. After giving their SBET areas and other details, it will be shown how to determine their wavelength dependent photocatalytic activities, and in one case (In_2S_3) a detailed mechanism of its action in the degradation of the RhB dye will be explained. It will be shown as well how to modify them in order to extend their wavelength range of activity (as is the case, for example, in the intermediate band scheme), and how photocatalytic and photoelectrochemical techniques can be used, combining these sulphides with some enzymes of types hydrogenase (with a bimetallic Ni-Fe cluster as active species) or laccase (having 4 Cu ions as active species), so as to achieve the photo-splitting of water. Preliminary results on the reduction of CO_2 to formate ions, using a formate dehydrogenase enzyme containing W as active element, will be shown as well

Title: Cooperative binding mechanism is the core of co–transport catalyzed by melibiose transporter MelB

LAN GUAN
Texas Tech Univeristy Health Sciences Center, USA

Biography:

Lan Guan, MD, PhD, Professor and Interim Chair, Department of Cell Physiology and Molecular Biophysics, and Director, Center for Membrane Protein Research, School of Medicine, Texas Tech University Health Sciences Center, Lubbock, Texas, USA. Her research has been funded by federal grants with a focus on molecular mechanisms of ion-coupled nutrient transporters using X-ray crystallography, single-particle cryo-EM, ligand binding thermodynamics, genetic engineering, and many other biochemical & biophysical analyses. Her laboratory determined the first 3-D high-resolution crystal structure of a Na+-coupled major facilitator superfamily transporter. She published 91 peer-reviewed research articles, reviews, and book chapters.

Abstract:

Secondary active transporters contain a large group of symporters that utilize the free energy installed in an electrochemical ion gradient across the cell membranes to catalyze uptake of varied solutes. Co-transport of solutes with cations is obligatory, but the principles underlying the cotransport is not well understood. We used a model system, the bacterial melibiose symporter MelB that couples melibiose uptake with the entry of H+, Na+, or Li+, to study Na+-coupled symport mechanisms. By determining high-resolution crystal structures of MelB and analyzing ligand binding, thermodynamics, and transport kinetics, it could be concluded that cooperative binding mechanism is the core of co-transport. It regulates the function of the transporter and ensures the obligatory symport. The positive cooperativity between the driving cation and driven substrate allows the transporters to catalyze uptakes effectively in substrate-limited environments.

Title: Metallic Membranes for Highly Intensified Ammonia Synthesis

Simona Liguori
Clarkson University, USA

Biography:

Simona Liguori is an Assistant Professor of Chemical & Biomolecular Engineering at Clarkson University and faculty affiliate at the Institute for a Sustainable Environment. She received her PhD and MS degrees in Chemical Engineering from University of Calabria (Italy). She continued her research at the Institute on Membrane Technology (ITM-CNR) - the Italian National Lab - as a Post-Doc researcher and in 2014 she joined Stanford University as a Physical Science Research Associate.
In 2016, she was appointed as Research Assistant Professor at the department of Chemical and Biological Engineering at Colorado School of Mines and, in 2018, she continued her career at Worcester Polytechnic Institute in the department of Chemical Engineering, where she received a Worcester Polytechnic Institute's Women's Young Investigator Fellowship and Carbon Footprint Challenge Award. In 2020, she was named a Scialog Fellow for Negative Emissions Science.

Abstract:

The world's primary energy sources are currently fossil fuels, including coal, oil and natural gas. Although society has benefited from the steady use of energy, continuing to use fossil fuels at such rates could lead to dire consequences. This motivates the development of new processes and technologies to produce carbon-neutral energy that breaks linear scaling relations while critically addressing environmental needs.
Ammonia (NH_3) is an important raw material for fertilizer production and today it is gaining attention as a new energy carrier for hydrogen (H_2). Ammonia represents the best carrier among the indirect hydrogen storages such as methanol, and methylcyclohexane, due to the zero CO_2 emission related to its decomposition. Also, ammonia is safer to transport than hydrogen. Conventionally, ammonia is synthesized through the well-known Haber-Bosch process at 400-500 °C and at pressures up to 300 bar. The high temperature, necessary for rapid kinetics, restricts conversion to ~20 percent. As a result, the recovery of NH_3 from the reactants is a critical unit operation in production plants. A series of heat exchangers and a final refrigeration stage are used to recover NH_3, while the remaining gases are reheated and recycled to a catalytic converter. In addition, the process requires fossil fuels and is, by itself, responsible for 2–3% of global carbon dioxide emissions.
Here, an intensified process using a 'smart' reactor (aka membrane reactor) is proposed to produce H_2, from methane steam reforming, and NH_3 in the same system at lower operating conditions than the traditional process. In addition, the system allows for the separation of a highly concentrated stream of carbon dioxide, which can be captured to address environmental issues. Laboratory data suggests that this technology is promising for innovative NH_3 synthesis processes operating at reduced conditions while paying attention to the environment.

CATALYSIS WEBINAR

SCIENTIFIC SESSIONS
(DAY 02)

SCHOLARS INTERNATIONAL WEBINAR ON

CATALYSIS, CHEMICAL ENGINEERING & TECHNOLOGY

NOVEMBER 25-26, 2021
ONLINE | VIRTUAL

Title: Carbon-silicon hybrid as anode material in energy sources

Marita Piglowska
Poznan University of Technology, Poland

Biography:

Eng. Marita Pigłowska (graduated in 2021), current master student of Composites and Nanomaterials at Poznan University of Technology. In her scientific carrier she published 9 articles in international reviewed journals. She took part in 2 international conferences (presented topics: flammability of lithium-ion cells (she won the prize for the best student oral presentation) and use fuel cells and batteries in automotive industry). In 2019 she became the winner of the 2nd place in Hydrogen Competition in Poland. In 2021 she won the Veolia contest for the best engineering thesis and took part in Summer School of Veolia.

Abstract:

Graphite is a commonly used active material in the anode of a lithium-ion cell. Its biggest disadvantage is its limited specific capacity, which is 372 mAh g-1. For this reason, more effective electrode materials have been sought for many years - incl. oxide with transition elements, carbon, silicon. In a lithium-ion cell, a capacity is sought, which is achieved by pure lithium, which cannot be used as an anode due to its danger and cost. Due to the great interest in green chemistry and an attempt to reduce waste from various industries, attempts are made to apply carbon materials. As it is not possible to achieve all valuable properties with the use of one material, composite and hybrid materials are used. Hybrid materials can be defined as combinations of two (or more) materials, of materials and space and composites are connected at the nanometer or molecular level. They are assembled in such a way as to have attributes that are not offered by any material separately. Using materials of natural origin increases the biodegradability of the cell, contributes to spreading the slogan of green chemistry, and also achieves high specific capacities after many charge-discharge cycles. Silicon, in general, presents high specific capacity, proper working potential, abundant availability, environmental friendliness. Unfortunately, there are some disadvantages such as huge volume change, unstable SEI, low conductivity, which could be fixed using natural carbon materials (biomass-derived) in hybrid systems, which is the main focus of this work.

Featured Speaker
CATALYSIS WEBINAR 2021

Title: Copolymers of poly(propylene fumarate) with phosphonic acid-based monomers designed as bone tissue engineering scaffolds

Erde Can Safak
Yeditepe University, Turkey

Biography:

Dr. Erde Can Şafak is an Assoc. Prof in the Chemical Engineering Department at Yeditepe University located in İstanbul, Turkey. Dr. Can recieved her Ph.D. in 2005 from University of Delaware in Materials Science and Engineering. She has expertise in the field of polymeric and composite materials in which she published several referred journal articles.
Research Interest: Polymers and composites from renewable resources, thermosetting polymers, polymeric biomaterials, polymer electrolyte membranes for fuel cells, polymer structure property relationships.

Abstract:

In order to heal a damaged bone, a biodegradable material which serves as a structural support to the damaged area and also acts as a scaffold that guides bone formation and enhances bone regeneration is a desirable solution. Polypropylene fumarate (PPF); an unsaturated polyester that can be cross-linked with suitable vinyl monomers to give biodegradable and biocompatible network structures is a candidate material to be used as a bone tissue engineering scaffold. In this study, hydroxyl terminated PPF was synthesized and thermally cured with changing amounts of vinyl phosphonic acid (VPA) and diethyl vinyl phosphonate (VPES) in the presence of radical initiator benzoyl peroxide (BP). Synthesized PPF was also cured with VPES at body temperature (37oC) using BP and a catalyst with varying amounts of Beta-tricalcium phosphate (ß-TCP) to prepare composite materials that can be used in injectable forms. Thermomechanical and compressive properties, biodegradability and hydrophilicity of the PPF/VPA and PPF/VPES copolymers were determined and evaluated with respect to composition. Biocompatability of the resulting polymers was determined by MTS assay and osteoblast activity was evaluated with von kossa, alkaline phosphatase and osteocalcin activity analysis. Different compositions of the thermally cured PPF copolymers exhibited compressive modulus and strength values in the wide range of 10–836 MPa and 14–119 MPa respectively. MTS assay showed that all the tested compositions were biocompatible and overall results of the study indicated that copolymers of PPF with VPA and VPES and their ß-TCP composites show serious potential as scaffolds for bone tissue engineering applications.

Title: Mechanical properties and environmental degradation in high strength aluminum alloys

Christian Paglia
Supsi imc, Switzerland

Biography:

Christian Paglia Ph. D in Material Science at the Swiss Federal Institute of Technology, in collaboration with Sika AG in Zurich. Post-doctoral Researcher at the Fontana Corrosion Center in the Corrosion of Aerospace Aluminum Alloys Friction Stir Welds at the Material Science Department, Ohio State University, Columbus, USA, in collaboration with the Wright Patterson Air Force Research Laboratories. Responsible of a branch office of the Helbling Consulting Engineering Group, Zurich. Director of the Institute of Materials and Constructions at the University of Applied Sciences of Southern Switzerland. Several publications on concrete, metals and other materials. Editorial board member of materials and corrosion scientific journals. Member of the SIA commission 215 on mineral binders. Member of the commission for the evaluation of the impartiality of the Swiss certification body for construction products S-CERT AG (CH) / S-CERT FL GmbH (FL)..

Abstract:

High strength aluminum alloy are used in the aircraft industry. The metal alloys are exposed to severe condition, alternatively varying in temperature and exposition to aggressive environment. The 7075-T651 and 7050-T7451 aluminum alloy represent some of the alloys used. Therefore, their mechanical properties and environmental degradation must be clearly investigated. This was carried out in this work by testing the alloys in the different tempers and by alternatively exposing them to a variation in temperature and in the aggressive environment, such as 20oC and 65% relative humidity, to a 3.5 weight % NaCl solution and by refrigeration at -20oC. The aluminum alloy in the annealed condition exhibits higher elongation as compared to the T-651 and T-7451 temper. The mechanical properties reach 500 Mpa. The T-651 temper exhibits a significant reduction in strain. Similar deformation but lower strength for the T-7451 temper as for the T-651 is observed. The environmental susceptibility of the 7075-T651 and 7050-T7451 at 20 oC is generally high with the alternate exposure to NaCl solutions and dry atmosphere (ductility ratio 0.5 to 0.7) respectively, while is generally reduced by the alternate exposition at low temperature because of the reduction of localized corrosion and initiation failure sites.

Title: Highly efficient dual step-scheme Bi2WO6/Fe2O3/WO3 heterojunction for the photodegradation of bisphenol-A

Pooja Shandilya
Shoolini University, India

Biography:

Pooja Shandilya is currently an Assistant Professor of School of Advanced Chemical Sciences at Shoolini University of Biotechnology and Management Sciences Solan, H.P., India. She has been working in the field of photocatalysis to develop novel heterojunction possessing broad absorption range and highly efficient for photocatalytic water detoxification and other environmental applications. She is exploring various metal oxide, layered double hydroxide, and carbon-based photocatalytic heterojunction having different type of charge migration that can be theoretically and experimentally characterized by DFT, XPS, ESR, and AFM technique and also by performing trapping experiments. The major aim of her studies is to construct sustainable and advanced nanomaterials for various photocatalytic applications. She has published nearly 28 SCI journal articles with 1789 citation in the area of material chemistry.

Abstract:

An efficient, visible light active, non-toxic, magnetically separable, and highly efficient charge separation dual step-scheme (S-scheme) Bi2WO6/Fe2O3/WO3 (BFW) heterojunction were designed by ultrasonic-assisted wet impregnation method. The morphology, chemical states, surface area, optical and electrochemical characteristics were examined by SEM, TEM, EDX, FTIR, BET, XRD, UV-Vis-DRS along with PL analysis. Different direction of charge migration follows S-scheme pathway that synergistically facilitates recoupling of useless charge carrier at heterojunction interface. The charge transfer and separation, mineralization process, and S- scheme type charge migration in BFW photocatalysts were in-depth investigated by electrochemical studies, HPLC, LC-MS, and XPS analysis. The superoxide and hydroxyl radicals generated on BFW heterojunction photodegraded 99% of bisphenol-A under visible light. The trapping experiments and ESR techniques were explored to establish the role of primary active species.

Moreover, the effect of catalyst dosage, BPA concentration, initial pH, and the presence of inorganic anions was also investigated. As reflected in VSM analysis, the strong-magnetic behaviour enables the heterojunction magnetically separable and recyclable up to 7 catalytic runs. Significant photocurrent density and lower charge transfer resistance at the interface demonstrate BFW as highly efficient photocatalysts for BPA degradation. Hence we believe this work furnish new insights for fabricating a novel S-scheme based heterojunction for environmental remediation.

Title: Polysaccharide chemistry and rheology

Jie Gao
University of Oklahoma, USA

Biography:

Jie Gao's current research focuses on functionalizing and manufacturing advanced materials for energy and water applications. These works include controlling porous morphology of polymer-based materials for membranes, functionalizing polysaccharide for improved rheological properties, as well as developing processes to make well-defined polysaccharide microparticles. One of her major research directions is water treatment. She has expertise in detecting organic and inorganic species in water as well as removing those undesired using state-of-the-art techniques. Leveraging the fundamental knowledge gained in the labs, she also developed industrial-scale procedures and equipment.

Abstract:

Natural polysaccharides are the macromolecular polymers obtained from sustainable sources such as plant and organism. The abundance of polysaccharide determines its economic value as a renewable resource. The molecular weight of guar gum is the highest of all known natural polymers produced of industrial gums, which enables this water-soluble polysaccharide to produce highly viscous solutions at low polymer concentrations. It can be a suitable replacement of some synthetic polymers due to low production cost and biodegradation capability. Guar thus plays a crucial role in the oil field, food, pharmaceutical and cosmetic industries, and chemical modifications will be valuable for further enhancing its performance. Here we explored efficient procedures like carboxymethylation and hydroxypropylation to modify and change their properties such as improved solubility and stability. The chemistry processes were specifically developed for guar splits. NMR spectroscopy and wet chemistry method were applied to quantify the conversion as a function of reaction time. For the first time, kinetic models were proposed, enabling the derivation of a reaction rate law for guar modification. In addition, borate and zirconium cross-linkers were applied to study the effect of cross-linking on the product, establishing a relationship between the structure and the rheological properties. The understanding from the studies laid the foundation for an engineering design to functionalize guar splits and broaden its industrial applications.

Title: Kinetic selection in the out-of-equilibrium autocatalytic reaction networks that produce macrocyclic peptides

Xiaoming Miao
Wuxiapptec, China

Biography:

Dr. Miao is now an associate principal scientist in WuXi Apptec, who did his postdoc in Weizmann Institute of Science in the field of autocatalysis and origin of life. He endeavored to design and construct the first chemical system where polymerization of peptide monomers results in predominantly macrocyclic oligomers. Further, Dr. Miao tried to understand how the combination of autocatalysis, diversity of products, and out-of-equilibrium conditions (open system) results in the selection of more functional using his knowledge in mathematic modeling of the reaction kinetics and flow chemistry. Dr. Miao obtained his Ph.D. in University of Groningen, working on selective fictionalization of the surface of nanoparticles and dendrimers using dynamic combinatorial chemistry.

Abstract:

Autocatalysis is considered central to the problem of the origin of life on Earth because it is a key ingredient of Darwinian evolution. However, not every type of autocatalysis can drive evolution. It requires competition between selectively self-amplified, information-carrying replicators. Molecular replicators (e.g., trinucleotides) often have complex structures that it is difficult to imagine their formation in considerable amounts in prebiotic environments. It is well understood how the selection of specific molecules occurs in reaction networks driven by template-assisted ligation; however how selection could occur in strongly interconnected, nonselective, autocatalytic networks is less clear. Here, we demonstrate that dimeric thioesters of tripeptides with the general structure (Cys-Xxx-Gly-SR)2 form strongly interconnected autocatalytic reaction networks that predominantly generate macrocyclic peptides up to 69 amino acids long. Some macrocycles of 6-12 amino acids were isolated from the product pool and were characterized by NMR spectroscopy and single-crystal X-ray analysis. We studied the autocatalytic formation of macrocycles in a flow reactor in the presence of acrylamide, whose conjugate addition to thiols served as a model “removal” reaction. These results indicate that autocatalytic production and competing removal of molecular species in an open compartment could be a feasible route for selecting functional molecules during the pre-Darwinian stages of molecular evolution.

Title: Enhancement of photoelectrochemical performance of (CCTO) using different nanosheets, graphene oxide and boron nitride

Sara Kawrani
Lebanese American University, Lebanon

Abstract:

Photoelectrochemical water splitting under visible light has attracted attention for renewable hydrogen production. Despite prevalent investigations, many challenges still hindered an efficient energy conversion, such as enhancing the reaction efficiency in visible light. Thus controlling the photoelectrode materials is an essential step in designing new materials for water splitting. $CaCu_3Ti_4O_{12}$ (CCTO) has received great attention as photocatalyst under solar light due to its combined band gap as result of the presence in its structure of TiO_2 active in UV light and CuO active under visible light. Physico-chemical characterizations demonstrate that bore and nitrogen co-doped CCTO causes an increase in grain boundaries thickness, and that the oxidation of GO at high temperatures lead to the reduction of Ti^{4+} to Ti^{3+} and Cu^{2+} to Cu^{+}, causing a segregation of copper on grain boundaries regions. The electrochemical performance of CCTO with Boron nitride and graphene oxide is investigated and showed that 3% of nanosheets lead to an increase in the generated current. Hydrogen production measurements show that the rate of H_2 production reached arround 8.1 µmol/h under visible light after adding 3% of BN nanosheets to CCTO which presents 16 times increase in comparison with pure CCTO. CCTO prepared using 3% of GO showed 50% higher photocurrent generation and hydrogen generation rate than pure phase of CCTO.

Title: Designing a multi-material nerve graft utilizing novel biofabrication techniques to promote peripheral nerve regeneration in injuries greater than 5 cm

Cayleigh O'Hare
Illinois Mathematics and Science Academy, USA

Biography:

Cayleigh O'Hare is a senior attending the Illinois Mathematics and Science Academy in Aurora, Illinois. She hopes to apply her experience in the field of materials science to restore use in injured neural tissue and eliminate the need for donor transplants. As a part of exploring how biomaterials can positively impact quality of life, Cayleigh conducts research as an intern at the Chicago-based biofabrication company Dimension Inx. With her studies, she aims to learn more about how the porosity of levels of graphene and various polyester polymers can make new advances in the field of tissue and organ regeneration.

Abstract:

Over 20 million people in the United States have peripheral nerve injuries. Additionally, these injuries result in approximately $150 billion spent in annual health-care dollars in the United States. For those living with peripheral nerve injuries spanning over 5 centimeters, treatment options can be especially elusive, and quality of life can be dramatically altered. With a nine-month literature review spanning hundreds of journal articles and publications, as well as interviews with multiple experts in the fields of materials science and neurosurgery, a novel theoretical peripheral nerve conduit was designed to induce optimal axonal regeneration. Market requirements for an optimal peripheral nerve graft include that it must promote neural regeneration, be surgically friendly, have a broad availability in a consistent form, be biocompatible, and eliminate donor site pain. Based upon the literature review and expert interviews, the following design inputs were established. Outer material of the conduit would be comprised of the polyester polymer polycaprolactone, or PCL, extruded through a 3-D printer into a scaffold. PCL is biodegradable and has been demonstrated to not trigger an immune response in the body. The unique nanostructure of the conduit would contribute to the conduit's high porosity; elevated porosity has been shown to promote cell adhesion, viability, and proliferation. Graphene would comprise the inner layer of the conduit, as its highly electroconductive properties are conducive to better neural cell communication and has demonstrated biocompatibility. Product specifications and prototype design were generated to account for these design inputs. Continued research would include prototype construction and design validation through preclinical testing. Future directions may include addition of growth factors to the conduit to further accelerate regeneration.

Featured Speaker
CATALYSIS WEBINAR 2021

CATALYSIS WEBINAR

Title: Heterogeneous Oxidation Catalysis: A Sustainable Route for Fine Chemical Production

Sourav Biswas
State University of New York, USA

Biography:

Sourav is from Kolkata (known as 'city of joy'), India and completed his Masters from Indian Institute of Technology Madras. He moved to the United States in 2011 to pursue his Ph.D at the University of Connecticut under Prof. Steven L. Suib. Sourav's interest in the field of catalysis and material chemistry bloomed during his Ph.D, when he studied a unique type of nanomaterials, recognized as 'University of Connecticut' or 'UCT' materials. Sourav pursued his postdoctoral study under Prof. Shannon S. Stahl at the University of Wisconsin-Madison, where he utilized his material synthesis skills on developing a 'flow-cathode' based fuel cell technology as an alternate energy source. Before joining Buffalo State, Sourav was appointed as a postdoctoral researcher at the Catalysis Center of Energy Innovation at the University of Delaware, where his project was to investigate the surface of metal nanoparticles by spectroscopic techniques.
Sourav has started his independent research career at the SUNY Buffalo State from Spring 2021.
Apart from research and teaching, Sourav likes to travel and spend time with his family and friends. He has visited 10 national parks (here in USA) so far with a goal of visiting all 63 parks. Below are some of the pictures of him at different travel destinations.

Abstract:

Selective oxidation of organic molecules by molecular oxygen is a subject of considerable importance in the context of the environmentally benign synthesis of commodity chemicals. Heterogeneous materials have been established as fundamental pillars supporting the advances in ‘green chemistry’, from the perspective of cost and waste minimization. However, dependability on precious metals, promoters/ additives and harsh reaction conditions hinder the widespread use of heterogeneous catalysts over traditional pathways for chemical synthesis. This talk will introduce some of the fundamental and practical challenges facing this field, together with a presentation of efforts we have made to address these challenges, emphasizing the development of a unique type of mesoporous transition metal oxide and its application in a series of selective oxidation reactions. This will be followed by understanding the mechanistic aspects, especially the role of the surface oxygen species, oxygen vacancies and related oxygen transportation by the metal oxides.

Title: Heterogeneous Oxidation Catalysis: A Sustainable Route for Fine Chemical Production

Avinash B. Lende
National Tsing Hua University, Taiwan

Biography:

Dr. Avinash B. Lende is currently working with a company. He completed his PhD from Department of Chemical Engineering, National Tsing Hua University, Taiwan under the supervision of Prof. Chung-Sung Tan. He holds two master's degrees in organic chemistry and chemical engineering. Dr. Avinash has more than ten years of research experience and has been working on the development of new heterogeneous catalysts for the selective hydrogenation of aromatic ring. To this effect, he has also published several international research articles of high importance regarding the same. His research focused on the greener synthesis of heterogeneous catalysts and sustainable aspects of chemical reaction engineering.

Abstract:

This study demonstrates the direct hydrogenation of polyethylene terephthalate (PET) dissolved in 1,1,1,3,3,3-hexafluro-2-propanol (HFIP) to environmentally friendly polyester polyethylene-1,4-cyclohexanedicarboxylate (PECHD) using a Vulcan XC-72 supported Rh-Pt bimetallic catalyst synthesized via a polyol method. The hydrogenation of PET was promoted by RhOx species present on the catalyst support surface which was generated using the polyol synthesis method. As compared to the monometallic Rh catalyst, the Rh-Pt bimetallic catalyst was found to be superior for hydrogenation of PET. This superiority was attributed to the strong aromatic ring adsorption ability of Rh working in synergy with an increased H2 spillover by Pt. At a H2 pressure of 1000 psi and 50 oC for 60 min, complete hydrogenation of PET to PECHD was achieved over the Rh-Pt bimetallic catalyst possessing theoretical Rh and Pt metal loadings of 2.5 wt% each. PECHD was found to be recovered to a very high extent using the compressed CO2 anti-solvent technique after hydrogenation of PET.

Title: Asymmetric Reduction of Carbonyl on Clean and Chirally Modified Single Crystal Model Pd and Pt Catalysts

Sree Pradipta Roy
University of Wisconsin Milwaukee, USA

Abstract:

The enantiomerically pure compound is required for pharmaceuticals and agrochemicals. In terms of separation and continuous production processes, heterogeneous phase chiral catalysts are suitable than homogeneous phase catalysts. Transition metals such as Pd and Pt are efficient hydrogenation catalysts for producing chiral compounds. In presence of a chiral modifier such as 1-(1-naphthyl) ethylamine (NEA) on catalysts surface, the mechanism by which chirality is happening is still an ongoing question. Over the past few decades, heterogenous asymmetric catalysis has drawn much attention for the enantioselective reduction of molecules containing ketone. Surface science study (10-7 ~ 10-10 Torr pressure) showed that prochiral reactants such as Methyl Pyruvate and Acetophenone can adsorb as pro-R or pro-S configuration on Pd and Pt surface modified by 1-(1-naphthyl) ethylamine (NEA). It leads us to find the answer to the question "is this chirality induced on adsorption preserved in the hydrogenation products? To investigate this, we carried out the catalysis (~ 760 Torr pressure) of hydrogenation reaction on single-crystal model Pd and Pt catalyst as same as the surface science studies. Our study on the reaction mechanism showed that hydrogenation reaction was going on via enol tautomer. Another important question is "does the reaction proceed on the NEA-covered catalyst surface and is it stable?". Therefore, we examined the effect of chiral modifier NEA on catalysts, and hydrogenation reaction was performed successfully.

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