UNITED Scientific Group
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CATALYSIS
February 22-26, 2022 | Hybrid | San Francisco, CA

6TH INTERNATIONAL CONFERENCE ON

Catalysis and Chemical Engineering

22-26
FEBRUARY, 2022
HYBRID SAN FRANCISCO, CA

Venue:
DoubleTree by Hilton
San Francisco Airport, 835 Airport Blvd.
Burlingame, CA

catalysis@uniscigroup.org

https://catalysis.unitedscientificgroup.org/

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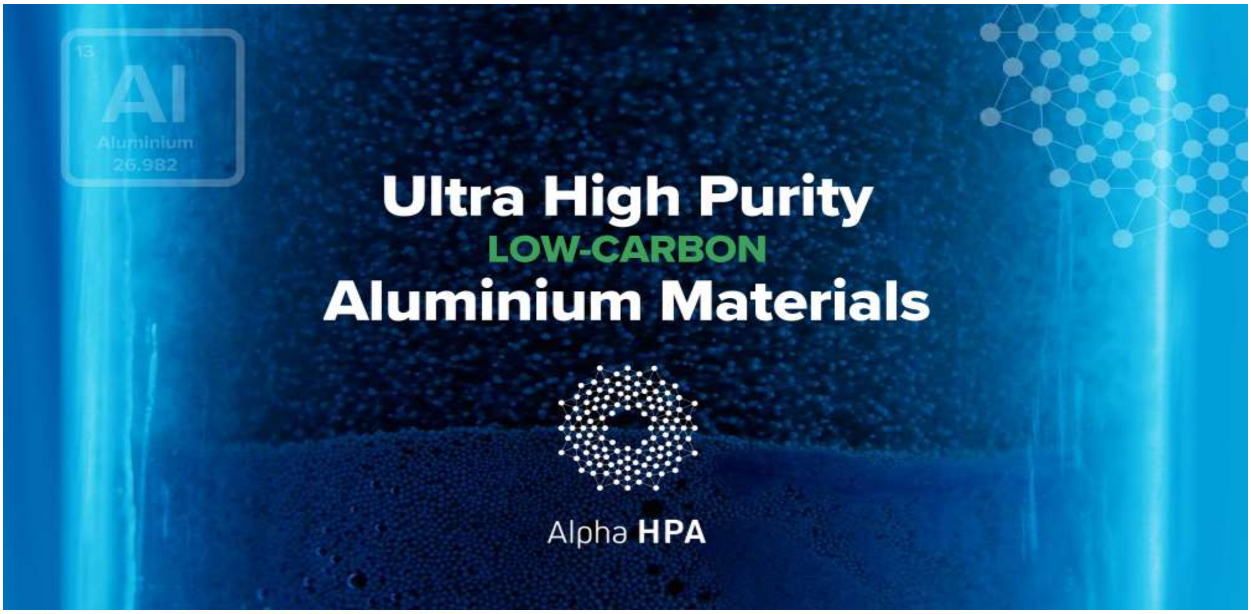

Introducing Alpha HPA

- Australian public listed materials processing and technology company
- Proprietary low carbon process for extraction and refinement yielding low cost, high purity alumina and hydrate salts.
- Pilot/Intermediate scale volumes available from Alpha HPA existing facility in Brisbane.
- Pathway to a large scale commercialization process as the "HPA First Project" by late 2022 and producing up to 10,000 tons of HPA equivalent per annum by late 2024.
- On commercialization, the HPA First Project is expected to be the largest HPA production center globally, delivering custom, premium high purity aluminum products

First Project: Ultra High-Purity Aluminium Product Offering

High Purity Aluminium Pre-cursors

$Al(NO_3)_3.9H_2O$
Ultra Aluminium Nitrate

Our >99.999% (5N) purity aluminium nitrate is the purest product available at commercial scale. Key applications in particle coating, LED, aluminate scintillators and other specialty products.

$Al_2(SO_4)_3.xH_2O$
Ultra Aluminium Sulfate

Our >99.999% (5N) purity aluminium nitrate is the purest product available at commercial scale. Key applications in particle coating, LED, aluminate scintillators and other specialty products.

High Purity Aluminas

Al_2O_3
Ultra High Purity Alumina Powder & Tablets

>99.995% (4N5) purity alpha & gamma HPA engineered to suit customers specifications such as bespoke particle sized powders, sintered and un-sintered granules and sintered custom ingots.

Al-O-OH
Ultra Boehmite

A bespoke engineered >99.995% (4N5) purity Boehmite to suit specific customer requirements, ideal for LiB separator coatings. Includes high dispersible boehmites for sol-gel applications

RHINELAND SPECIALTIES
Specialty intermediates and additives

Alpha HPA

http://rhinelandspecialties.com

http://www.alphahpa.com.au

IN-PERSON MEETING GUIDELINES

COVID-19 safety policies:

The health and safety of all our participants remains our top priority. We are closely monitoring government mandates and policy changes, Centers for Disease Control and Prevention (CDC) guidelines and public health advancements (https://www.cdc.gov/).

Face-coverings

Wearing mask is recommended in the meeting premises / in-doors.

Hand sanitizer stations

Hand and washing facilities and/or sanitizing systems easily accessible to everyone throughout the event.

No contact policy

To assist in minimizing potential physical contact, elbow bumps are a great alternative to handshakes.

Presentations (PPT/PPTX/PDF)

To avoid physical contact, we request all the in-person presenters to submit the presentation at: https://catalysis.unitedscientificgroup.org/submit_presentation

WiFi

WiFi network and pass code will be shared on arrival to the meeting room.

Q & A

Moderator/Chair will pick up questions from the audience in the meeting room (at venue) and also from the zoom chat function – and ask the speaker to answer live.

MEETING JOINING LINKS (LIVE STREAMING ON ZOOM PLATFORM)

PACIFIC TIME

As the conference is hybrid, the virtual attendees can access the in-person presentations and queries can be asked through zoom chat box.

Meeting links shared will be for the complete meeting to join at any point of time.

February 22-26, 2022 – Room 1

Topic: VI International Conference on Catalysis and Chemical Engineering | February 22-26, 2022 | San Francisco, CA | Hybrid | Room 1

Join Zoom Meeting
https://us02web.zoom.us/j/83449413825?pwd=dk5DQk9ibTFBczdvbjM2YWpvSFRxdz09
Meeting ID: 834 4941 3825
Passcode: 224460

February 24-25, 2022 – Room 2

Topic: VI International Conference on Catalysis and Chemical Engineering February 24-25, 2022 | San Francisco, CA | Hybrid | Room 2

Join Zoom Meeting
https://zoom.us/j/92295987408?pwd=aTJSQjMwcXZrUnRXbnRiR0RxYjNpZz09
Meeting ID: 922 9598 7408
Passcode: 420436

DAY 01

FEBRUARY 22, 2022

IN-PERSON | ROOM-1: SIERRA-A

ROOM-1: SIERRA-A

PACIFIC TIME

Join the meeting
https://us02web.zoom.us/j/83449413825?pwd=dk5DQk9ibTFBczdvbjM2YWpvSFRxdz09
Meeting ID: 834 4941 3825
Passcode: 224460

07:30-07:50	Registrations and Badge Pickup	@ Fire Place Side
07:50-08:00	Opening Ceremony	

Plenary Presentations @ SIERRA-A

Moderator: Johan G. Alauzun, Université de Montpellier, France

08:00-08:40

Toward a Circular Plastics Economy. Catalytic Approaches to Polyester Deconstruction

Tobin J. Marks, Northwestern University, Evanston, IL

Prof. Tobin Marks is Ipatieff Professor of Catalysis and Materials Science and Engineering at Northwestern U. He holds a BS from the U. of Maryland and a PhD from MIT. Recognitions: U.S. National Medal of Science, ACS Priestley Medal, Spanish Asturias Prize, MRS Von Hippel Award, Dreyfus Prize in Chemical Sciences, NAS Award in Chemical Sciences, CAS President's International Distinguished Scientist Award, Israel Harvey Prize. Membership: U.S., European, German, Italian, and Indian Academies of Science, U.S. NAE and NAI, American Academy of Arts and Sciences; RSC, MRS, ACS, AIC Fellow. Research interests: unconventional catalysis, soft and hard matter electronic materials, and photovoltaics.

08:40-09:20

Atomistic Mechanisms of Heterogeneous-, Homogeneous-, and Electro-catalysts from QM and QM

William Andrew Goddard III, California Institute of Technology, Pasadena, CA

Prof. William Andrew Goddard III is currently Charles and Mary Ferkel Professor of Chemistry, Materials Science, Appl. Physics at California Institute of Technology (Caltech), Pasadena, CA. He is Director of Materials and Process Simulation Center (MSC). He has been a pioneer in developing methods for quantum mechanics (QM), force fields (FF), reactive dynamics (ReaxFF RD), electron dynamics (eFF), molecular dynamics (MD), and Monte Carlo (MC) predictions on chemical, catalytic, and biochemical materials system. He is a member of the International Academy of Quantum Molecular Science and the U.S. National Academy of Sciences.

Keynote Presentation @ SIERRA-A

09:20-09:50

Control of Functional Soft Materials

Monica Olvera de la Cruz, Northwestern University, Evanston, IL

Prof. Monica Olvera de la Cruz obtained her B.A. in Physics from the UNAM, Mexico, in 1981, and her Ph.D. in Physics from Cambridge University, UK, in 1985. She was a guest scientist (1985-86) in the National Institute of Standards and Technology, Gaithersburg, MD. She joined Northwestern University in 1986, where she is the Lawyer Taylor Professor of Materials Science & Engineering and Professor of Chemistry, and by courtesy Professor of Chemical & Biological

Engineering, and of Physics and Astronomy. She is the Director of the Center for Computation and Theory of Soft Materials and Deputy Director of the Center for Bio-Inspired Energy Science. From 2006-2013 she directed the Materials Research Center at Northwestern. From 1995-97 she was a Staff Scientist in the Commissariat a l'Energie Atomique, Saclay, France, where she also held visiting scientist positions in 1993 and in 2003. She has developed theoretical models to determine the thermodynamics, statistics and dynamics of macromolecules in complex environments including multicomponent solutions of heterogeneous synthetic and biological molecules, and molecular electrolytes.

Oral Presentations @ SIERRA-A

Catalysis and Chemical Engineering

Chair: Sebastien Laulhe, IUPUI, Indianapolis, IN

09:50-10:10 **New Directions in Sustainable Chemistry: From Allylation to C-H Activation**
Gregory R. Cook, North Dakota State University, Fargo, ND

10:10-10:30 **Explorations of the Redox-Active Azothioformamide Ligand Class through Metal Complexation and Catalysis**
Kristopher Waynant, University of Idaho, Moscow, ID

10:30-10:45 Break @ SIERRA FOYER

10:45-11:05 **Novel Organic Photoredox Catalysts for Greener Functionalizations of Aryl Halides**
Sebastien Laulhe, IUPUI, Indianapolis, IN

11:05-11:25 **Multifunctional TiO_2 Nanorods Grown on Glassy Carbon Foam for Efficient Solar Vapor Generation**
Sungdo Kim, University of Ulsan, South Korea

11:25-11:45 **Copper Core - Silica Shell Supports for Cobalt Catalyzed Fischer-Tropsch Synthesis: Impact on Thermal Stability within a Packed Bed Reactor and Effects on Product Distribution**
Fred MacDonnell, The University of Texas at Arlington, Arlington, TX

11:45-12:05 **Clean Energy Nanocatalysts Made by Pulsed Laser in Liquids Synthesis**
Astrid Mueller, University of Rochester, Rochester, NY

12:05-12:25 **MOF-Derived $PtCo/Co_3O_4$ Nanocomposites in Carbonaceous Matrices as Highperformance ORR Electrocatalysts Synthesized via Laser Ablation Techniques**
Dibyendu Mukherjee, University of Tennessee, Knoxville, TN

12:25-12:45 **Study of Electricity Transport Mechanisms in some Ruthenate Pyrochlores**
Sepideh Akhbarifar, The Catholic University of America, Washington, D.C.

12:45-12:50 Group Photo @ SIERRA-A

12:50-13:35 Lunch @ 37 NORTH WINDOW SIDE

Chair: T. C. Mike Chung, Pennsylvania State University, State College, PA

13:35-13:55	**Synthesis of Long-Chain Branched Polypropylene (LCB-PP) Polymers Using Both Homogeneous and Heterogeneous Ziegler-Natta Catalyst** **T. C. Mike Chung**, Pennsylvania State University, State College, PA	
13:55-14:15	**Microfluidic Device (Tetherchip) with Lipid-Modified Polyelectrolyte Multilayer Nanosurface Enables Efficient Cell Capture and Microtentacle Fixation for Circulating Tumor Cell Analysis** **Stuart Martin**, University of Maryland School of Medicine, Baltimore, MD	
14:15-14:35	**A Coating Strategy for Hydrogen Production from Sunlight at Scale** **Shu Hu**, Yale University, New Haven, CT	
14:35-14:55	**Facilitated Hydrogenation of Aromatic Nitro Compounds Using Polymer-Supported Heterogenous Catalyst with Rhenium Nanoparticles** **Piotr Cyganowski**, Wroclaw University of Science and Technology, Poland	
14:55-15:15	**First Atomic Scale Evidence of Size Dependent Structural Transition of Hydrogenated Gold Nanoparticles: Toward A Realistic Picture of Reactive Surface** **Hazar Guesmi**, University of Montpellier, France	
15:15-15:35	**Intermetallic Monolithic Catalysts for Selective Hydrogenation of Phenylacetylene** **Pawel Czaja**, Polish Academy of Sciences, Poland	
15:35-15:50	Coffee Break	@ SIERRA FOYER

Chair: Enno Wagner, Frankfurt University of Applied Sciences, Germany

15:50-16:10	**Recyclable Pd-Based Polysaccharide Catalyst for Aerobic Oxidation of Benzyl Alcohol** **Adi Wolfson**, Sami Shamoon Collage of Engineering, Israel	
16:10-16:30	**Tunable Liquid Metal Complexes as Catalysts for the Model Chemical Processes** **Anna Chrobok**, Silesian University of Technology, Poland	
16:30-16:50	**Biophotocatalytic Wastewater Treatment System: CO_2 Methanation of Anaerobic Digester Biogas Using Magnetized Photocatalyst (Fe-Tio_2)** **Emmanuel Kweinor Tetteh**, Durban University of Technology, South Africa	
16:50-17:10	**Bifunctional Catalysts for Energy Storage with High-Efficient Fuel Cells** **Enno Wagner**, Frankfurt University of Applied Sciences, Germany	
17:10-17:30	**Temperature Effect on Hydrothermal Synthesis of Nickel Oxide Nanosheets as Electrocatalysts for Urea Electro-Oxidation** **Patrick Cognet**, Université de Toulouse, France	
17:30-17:50	**Novel Methods for Ammonia Synthesis** **Samira Siahrostami**, University of Calgary, Canada	
17:50-18:05	Coffee Break	@ SIERRA FOYER

Chair: Elisabeth Egholm Jacobsen, Norwegian University of Science and Technology, Norway

18:05-18:25	**Designing of Supported Ionic Liquid Phase Catalysts Dedicated for Aminolysis of Epoxides in Continuous Flow Synthesis** **Piotr Latos**, Silesian University of Technology, Poland

18:25-18:45	**Catalytic Metal-Hydride Regeneration from Metal-Alkoxides and Metal-Amidos** **Moris Eisen**, Technion, Israel	
18:45-19:05	**Chemo-Enzymatic Synthesis of Pure Enantiomers of β-Antagonists Esmolol and Penbutolol** **Elisabeth Egholm Jacobsen**, Norwegian University of Science and Technology, Norway	
19:05-19:25	**Stable Pt Nanoclusters on Mos_2 Slabs for Electrocatalytic Water Splitting** **Tamas Ollar**, Centre for Energy Research, Hungary	
19:25-19:45	**Solid State Electrocatalytic Processes Studied by a Novel Method Combining Impedance Spectroscopy with Transmission Electron Microscopy** **Saren Bredmose Simonsen**, Technical University of Denmark, Denmark	
19:45-20:05	**Synthesis Mesoporous Materials as Catalyst Support by Non-Hydrolytic Sol-Gel** **Johan G. Alauzun**, Université de Montpellier, France	
20:05-20:25	**Synthesis Temperature Dependence of ORR Activity in Catalysts Derived from CO_2 via Alkali Carbonate/Hydroxide Molten Salts** **Ivar Kruusenberg**, National Institute of Chemical Physics and Biophysics, Estonia	
20:25-21:00	**Poster Presentations**	**@ SIERRA-A**
CCEP-01	**Photocatalytic Decomposition of N_2O over Sulfure Doped G-C_3N_4 Photocatalysts** **Marcel Sihor**, Institute of Environmental Technology, Czech Republic	
CCEP-02	**Evaluation of Performance, Modeling and Simulation of Fenton Process in Reducing the Oil and Grease Content of Produced Water** **Marcellus Guedes Fernandes de Moraes**, Federal University of Rio de Janeiro, Brazil	
CCEP-03	**Biogenic Synthesis of Green Gold Nanoparticles for the Catalytic Reduction of Nitroaromatic Compounds** **Dorota Jermakowicz-Bartkowiak**, Wroclaw University of Science and Technology, Poland	
CCEP-04	**Removal of Endocrine Disruptors by Means Hybrid Membrane-Sorption Process** **Joanna Wolska**, Wroclaw University of Science and Technology, Poland	
CCEP-05	**The Potential of Using Nanocomposite Poly(Vinyl Chloride) Membranes With Au Nanoparticles for the Catalytic Reduction-Separation Process** **Joanna Wolska**, Wroclaw University of Science and Technology, Poland	
CCEP-06	**Manganese Ferrite/Graphitic Carbon Nitride Activated Peroxymonosulfate to Re move Steroid Hormone-Contaminated Water** **Chainarong Sakulthaew**, Kasetsart University, Thailand	
CCEP-07	**Magnetic $MnXCu_1$-XFe_2O_4 Nanoparticle as Visible Light Photo-Fenton Catalyst for the Removal of Organic Contaminants: Implication for Water Treatment** **Athaphon Angkaew**, Kasetsart University, Thailand	
CCEP-08	**Enhanced Catalytic Oxidation of Toxic Organic Pollutants by Metal Ferrite Nanocomposites Under Various Environmental Conditions** **Chanat Chokejaroenrat**, Kasetsart University, Thailand	
21:00-22:00	Dinner	@ 37 NORTH WINDOW SIDE

End of Day-1

PROGRAM

ZOOM PLATFORM VIRTUAL MEETING INSTRUCTIONS

Join the zoom meeting

Join the meeting by clicking on a Zoom meeting link provided by the meeting host => follow the prompts to download and run Zoom => enter the meeting ID if prompted => click to join the audio (OR) if you already have Zoom software installed in your system, simply open Zoom application, click 'join' and enter the meeting code.

Mute/unmute & audio settings

Except for the moderator and the speaker, all attendees' microphones will be muted by the host.

Chat function for Q&A

The participants will submit their questions through the chat box and the moderator/chair of the session will pick the questions for the discussion. Direct your question by tag the speakers name to the questions as you submit them to the chat (e.g., For Dr. Will Torres – Question 1).

Audience

We are anticipating over 300 attendees who will come from a range of professional backgrounds with a varied level of knowledge and expertise in technical and commercial aspects across the subject area.

For speakers

You will be allowed to share your screen during your presentation. Session moderator will pick the questions from the participants and asks the speaker depending on the time available. In case if more questions are left in the chat box, we encourage speakers to answer via chat and continue the discussion.

For poster presenters

All the poster presentation recorded videos are made available to all the participants to view at any point of time at their convenience. According to the program, the presenter will be available during the time slot for the Q&A.

Recording

The session will be recorded for training purpose and some for the video library. Most of the speakers have already consented to recording their presentation but please inform us otherwise if you have some content which should not be recorded.

If you have trouble in login or any technical issues, please write to contact@uniscigroup.net or call us at 469-854-2280.

DAY 02

FEBRUARY 23, 2022

VIRTUAL | ROOM-1

PROGRAM

PACIFIC TIME

Join the meeting
https://us02web.zoom.us/j/83449413825?pwd=dk5DQk9ibTFBczdvbjM2YWpvSFRxdz09
Meeting ID: 834 4941 3825
Passcode: 224460

05:50-06:00 Opening Remarks and Introduction

Moderator: Mannar Ram Maurya, Indian Institute of Technology Roorkee, India

Keynote Session-I

06:00-06:30

First-row Transition Metal Nanocatalysts: Design and Mechanistic Insights

Montserrat Gomez, University Toulouse, France

Montserrat Gómez received her PhD in 1991 (University of Barcelona, UB, Spain), in organometallic chemistry and homogeneous catalysis. She carried out a post-doc in the group of I. Tkatckenko (Toulouse, France, 1992) and sabbatical stays in the teams of P. van Leeuwen (Amsterdam, 1998) and B. Chaudret (Toulouse, 2002). In the period 1993-2004, she occupied a Lecturer position at the UB working on chiral ligands design and enantioselective catalysis. Since 2005, she is Full Professor at the University Paul Sabatier (Toulouse). Her current research goals focus on metal-based nanocatalysis using non-conventional solvents and functionalized supports, with special interest into mechanisms.

06:30-07:00

Dynamic Response of Metallic Catalysts Towards Reaction Conditions

Robert Schlogl, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany

Robert Schlogl studied chemistry at the Ludwig Maximilian University of Munich (LUM), Germany, where he received his Ph.D. in 1982. He then did postdoctoral research at the Universities of Cambridge, UK, and Basel, Switzerland. Schlogl completed his habilitation at the Fritz Haber Institute in 1989. The same year, he joined the University of Frankfurt am Main, Germany, as Full Professor of Inorganic Chemistry. Since 1994, Schlogl has served as Director at the Fritz-Haber-Institute and Honorary Professor at the Technical University of Berlin. He was also named Honorary Professor at the Humboldt University of Berlin in 1998. Since 2011, he has been Founding Director at the Max Planck Institute for Chemical Energy Conversion. He has also been named Honorary Professor at the University Duisburg-Essen, Germany, in 2012 and Honorary Professor at the Ruhr-University Bochum (RUB), Germany, in 2015. Among other honors, Schogl has received the DECHEMA-Plaque in 2010, the Alwin Mittasch Prize in 2015, and the Innovation Award 2015 from the Ministry for Innovation, Science, Research and Technology (MIWF) of the State of North Rhine-Westphalia, Düsseldorf, Germany. He serves on the Editorial Board of ChemCatChem and is a Fellow of the Royal Society of Chemistry (RSC).

07:00-07:30

Polymer Grafted Vanadium Complexes in Catalytic Organic Transformations

Mannar Ram Maurya, Indian Institute of Technology Roorkee, India

Mannar Ram Maurya is currently with the Department of Chemistry as a Professor of Inorganic Chemistry of Highest Academic grade and Dean of Faculty Affairs of Indian Institute of Technology Roorkee, India. He has also served as Chair of Department of Chemistry. He received his Ph.D. from Kurukshetra University (NIT, Kurukshetra), Kurukshetra, 1987 and M.Sc. from Bundelkhand University, Jhansi, 1981 and B.Sc. from Gorakhpur University, 1979. He has worked as a Lecturer in University of Pune from 1993-1996, Assistant Professor from 1996-2004, Associate professor from 2004-2008 and as a Professor in I.I.T. Roorkee from 2008-till now. He has more 6000 citations in his credit. He worked as a Guest Editor for Topics in Catalysis and Catalysis Today for Special Issues published based on the papers presented in 2nd, 3rd and 4th International Conference on Catalysis and Chemical Engineering, respectively.

07:30-08:00

Graphene-CNT Supported Metal Oxide Nanoparticles for Hydrogenation, Hydrodeoxygenation and Oxidation

Martin Schmal, Federal University of Rio De Janeiro, Brazil

Martin Schmal is Professor since 1970, became full Professor in 1985 and Emeritus since 2008 at the chemical engineering department of the Federal University of Rio de Janeiro and Professor at the University of S.Paulo since 2014. He is a Member of the Brazilian Academy of Science, elected in 1999 and of the International Catalysis Society since 2000.

08:00-08:30

Catalytic Conversion of Biomass to Fuels at NC A&T Bioenergy Center

Debasish Kuila, North Carolina A&T State University, Greensboro, NC

Debasish Kuila, previous Chair and Professor of chemistry, is the Research Director of NSFCREST Bioenergy Center at North Carolina A&T State University. He is also the Project Director of the University of North Carolina Research Opportunity Initiative. He was an associate professor at Louisiana Tech and spent over 10 years at Hoechst Celanese and Great Lakes Chemical Corporations and Purdue University. His research interest spans from materials/ biomaterials, cell biology, to catalysis. He received Chemcon Distinguished Speaker Award in 2019 in Jaipur, India. He has 12 US Patents/applications and has been invited as keynote and plenary speakers for several international conferences.

08:30-09:00

Polyoxometalate Catalysts for Ongoing and New Routes to Solar Fuels

Craig L. Hill, Emory University, Atlanta, GA

Craig L. Hill, the Goodrich White Professor at Emory University, has been studying catalysis, reaction mechanisms and materials science for years. Current research focuses on solar fuels, catalytic and multi-electron transfer processes, nanoscale materials and polyoxometalates. He has received three ACS awards, many others, is a Fellow of AAAS, the Victorian Institute of Chemical Sciences, the Academia Europaea, and the Royal Society of Chemistry. He has chaired NSF and NRC committees, several conferences, edited a journal and been a nominator for 1992-present Nobel Prizes in Chemistry. His H-index (GS) from Emory (95) + Berkeley (9) is 104.

09:00-09:10 Break

09:10-09:40

Functional Catalytic Profiling of Species Across Fungal Kingdom

Lene Lange, BioEconomy, Denmark

Lene Lange PhD and Post-doc positions at University of Copenhagen. Ministry of Foreign Affairs, Seed Pathology Institute, 1978-86. From 1987-2007, holding R&D positions in Novo, Novo Nordisk, Novozymes A/S, finishing in top research career-position (Director of Research, in Molecular Biotechnology). From 01.02.07, recruited back to academia, first as Head of Institute of Biology, University of Copenhagen; from 01.09.08 Dean of Research and Professor in Biotechnology at Aalborg University, Denmark; Campus Director, Aalborg University, AAU Cph, 2009-2013; Director of Research, Aalborg University 2012-2015. Professor and Research leader, Technical University of Denmark 2015-2018. From 2018, own startup company, BioEconomy, Research & Advisory.

09:40-10:10

Computational Chemistry Considerations Towards Transition Metal and Heavy Element Species

Angela K. Wilson, Michigan State University, East Lansing, MI

Angela K. Wilson is currently the John A. Hannah Distinguished Professor of Chemistry and Director of the MSU Center for Quantum Computing, Science, and Engineering at Michigan State University. She is also Associate Dean for Strategic Initiatives in the MSU College of Natural Sciences. From 2016-2018, Wilson was the Division Director (head) of the Division of Chemistry at the U.S. National Science Foundation. Her research includes the development of quantum mechanics and quantum dynamics methodologies as well as a broad range of applications including homogeneous and heterogeneous catalysis. Among her honors are the Francis P. Garvan-John M. Olin Medal (ACS), IUPAC Distinguished Woman in Chemistry, Wilfred T. Doherty Award, Fellow of ACS, APS, and AAAS. She is on the editorial advisory board of the *Journal of Physical Chemistry* and *Cell Reports Physical Chemistry*, as well as the editorial board of *Scientific Reports*. She is 2022 President of the American Chemical Society.

10:10-10:40

Quantum Nutcracker for Near-room-temperature H_2 Dissociation

Sokrates T. Pantelides, Vanderbilt University, Nashville, TN

Sokrates T. Pantelides received a Ph.D. in physics from the University of Illinois at Urbana-Champaign in 1973. He served as Research Staff Member, Manager, Senior Manager and Program Director at the IBM T. J. Watson Research Center. He joined Vanderbilt University as the McMinn Professor of Physics in 1994. In 2010 he was appointed University Distinguished Professor of Physics and Engineering. His research work is theoretical/computational and spans semiconductor physics, device physics, quantum transport in nanostructures, complex oxides, nanocatalysis, magnetic phenomena, and interactions of light with matter. He is a Fellow of APS, MRS, AAAS, and IEEE.

10:40-11:10

New Nanostructures for Increased Selectivity and Stability in Catalysis

Francisco Zaera, University of California, Riverside, CA

Francisco Zaera is presently a Distinguished Professor of Chemistry at University of California, Riverside, CA, a Cooperative Faculty Member of the Chemical & Environmental Engineering Department, a Participating Faculty of the Materials Science and Engineering Program, the Director of the UCR Center for Catalysis, and the Assistant Director for XPS of the UCR Analytical Chemistry Instrumentation Facility. He is also Senior Editor of The Journal of Physical Chemistry Letters. He has authored over 370 articles in scientific publications, and has received several international awards, including the American Chemical Society George A. Olah and Arthur W. Adamson Awards, the North American Catalysis Society Paul H. Emmett Award, and a Humboldt Research Award for Senior Scientists. He is a Fellow of the American Chemical Society, the American Vacuum Society, and the American Association for the Advancement of Science.

Oral Presentations-I

Synthesis

Chemical Synthesis | Pyrolysis | Enzymes & Biocatalysts

Chair: Thomas J. J. Mueller, Heinrich Heine University Dusseldorf, Germany

11:10-11:30 **Metal Dusting of Ni-m Alloys in Hydrocarbons Atmosphere: In Search of Effective Catalyst for Production of H_2 and Carbon Nanomaterials**
Afonnikova Sofya Dmitrievna, Boreskov Institute of Catalysis, Russia

11:30-11:50 **Ni- and Co-Based Nano-Alloyed Catalysts for H_2-Assisted CCVD of Trichloroethylene into CNF Material**
Arina Potylitsyna, Boreskov Institute of Catalysis, Russia

11:50-12:10 **DBU Catalyzed Enantioselective Synthesis of Quaternary 2-Aryl Amino Acid Derivatives**
Francesca Foschi, Università degli Studi dell'Insubria, Italy

12:10-12:30 **Palladium Coupling Chemistry for the Synthesis of Quinoline based Natural and Unnatural Products**
Magne O. Sydnes, University of Stavanger, Norway

12:30-12:50 **Catching Multiple Birds with One Stone – One Pot Synthesis of Functional Heterocycles by Sequentially Palladium-Catalyzed Processes**
Thomas J. J. Mueller, Heinrich Heine University Dusseldorf, Germany

12:50-13:20 Break

Chair: P. Shing Ho, Colorado State University, Fort Collins, CO

13:20-13:40 **Development of Novel Chemoenzymatic Route to Enantiomeric β-Adrenolytic Agents**
Pawel Borowiecki, Warsaw University of Technology, Poland

13:40-14:00 **Enzymatic Degradation of Chlorinated Aromatic Compounds: Catalytic Mechanism to Biomaterials**
Richard C. Holz, Colorado School of Mines, Golden, CO

14:00-14:20 **Hydrogen Bond Enhanced Halogen Bonds in Biomolecular Catalysis**
P. Shing Ho, Colorado State University, Fort Collins, CO

14:20-14:40 **Design and Use of a Pd/B-Dual Catalyzed Glycosylation for the De novo Synthesis of Oligosaccharide**
George A. O'Doherty, Northeastern University, Boston, MA

14:40-15:00 **Thermal Activation Barriers of Enzyme Catalyzed C-H Cleavage by Tunneling**
Adam Offenbacher, East Carolina University, Greenville, NC

15:00-15:20 **Harnessing Immobilized Enzymes for Biocatalysis**
Ming-Qun Xu, New England Biolabs, Ipswich, MA

15:20-15:40 **The Core Principle of Cation-Coupled Transport by Melibiose Transporter MelB**
Lan Guan, Texas Tech University Health Sciences Center, Lubbock, TX

15:40-15:50 Break

Chair: Francisco J. Rodriguez Valadez, Centro de Investigación y Desarrollo Tecnológicoen Electroquímica, Mexico

15:50-16:10	**Bio-Electro Catalysis for a Net-Zero Future** **Frauke Kracke**, Stanford University, Stanford, CA
16:10-16:30	**Operando Near-Surface Imaging of the Multi-Component Gas Phase above a Catalyst** **Jonathan Frank**, Sandia National Laboratories, Livermore, CA
16:30-16:50	**Chemo-Enzymatic Synthesis of Tumor-Associated Complex Gangliosides for Immunological Studies** **Chang-Chun Ling**, University of Calgary, Canada
16:50-17:10	**Catalytic Pyrolysis of Sewage Sludge for Producing Bio-Oil and Sludge-Based Activated Carbon (SBAC) for Capturing Emerging Contaminants** **Badr Ali Mohamed**, University of British Columbia, Canada
17:10-17:30	**Kinetic Studies of Transesterification Reaction to Produce Biodiesel Using a Pilot Scale Ultrasonic Reactor** **Francisco J. Rodriguez Valadez**, Centro de Investigación y Desarrollo Tecnológico en Electroquímica, Mexico
17:30-17:50	**Gold Mediated Arylation Reactions with Aryldiazonium Salts** **Susana Porcel Garca**, Universidad Nacional Autónoma de México, Mexico
17:50-18:00	Break

Keynote Session-II

Moderator: Richard C. Holz, Colorado School of Mines, Golden, CO

18:00-18:30

Using Speciation Chemistry to Change Enzyme Catalysis: a Case of Changing Phosphatase Specificity

Debbie C. Crans, Colorado State University, Fort Collins, CO

Debbie C. Crans is a professor of chemistry at Colorado State University, Fort Collins, CO. Her research interests includes Biological, Bioinorganic, Bioorganic and Bioanalytical Chemistries. She received her PhD from Harvard University and Postdoc from UCLA. She received many awards including 2019 ACS Award for Distinguished Service and Outstanding Research in the Advancement of Inorganic Chemistry, 2015 Arthur P. Cope Scholar award (Late Career) American Chemical Society, 2004 Vanadis Award, 2014 AAAS fellow and 2009 ACS fellow. She is also an Associate Editor of Coordination Chemistry Reviews and New Journal of Chemistry. She is Councilor for Division of Inorganic Chemistry, ACS. Chair-Elect: Colorado Section of ACS. Chair: Vanadis Award. Editorial Boards: Coordination Chemistry Reviews, Journal of Inorganic Biochemistry, New Journal of Chemistry. 2022 Chair, International Coordination Chemistry Conference.

18:30-19:00

Photocatalysis Mediated by Far-Red Light

Taniyuki Furuyama, Kanazawa University, Japan

Taniyuki Furuyama received his PhD in Pharmaceutical Sciences degree from The University of Tokyo in 2010, under the supervision of Profs. Masanobu Uchiyama and Yuichi Hashimoto. After working at RIKEN as a postdoctoral researcher and at Tohoku University as an Assistant Professor, he was appointed as an Associate Professor at Kanazawa University in 2015. His research interests include the synthetic chemistry of organic functional dyes and pigments toward the utilization of far-red-to-near-infrared light.

19:00-19:30

Silicon-Based Cross Coupling Reaction

Tamejiro Hiyama, Chuo University, Japan

Tamejiro Hiyama, Professor of Research Development Initiative, Chuo University. Bachelor of Engineering Kyoto University, March 1969, Master of Engineering Kyoto University, March 1971, Doctor of Engineering Kyoto University, September 1975, Postdoctoral Research at Harvard University, Sept. 1975-Aug. 1976 work with Professor Yoshito Kishi. 1972-1981 Associate Professor, Kyoto University, Faculty of Engineering 1981-1983 Research Fellow, Group Leader, Sagami Chemical Research Center 1983-1988 Senior Research Fellow, Group Leader, SCRC 1988-1992 Executive Research Fellow, Group Leader, SCRC 1992-1998 Professor, Research Laboratory of Resources Utilization, Tokyo Institute of Technology 1997-2010 Professor, Kyoto University 2010– Professor Emeritus, Kyoto University; RDI Professor, Chuo University. He has many awards including The Japan Liquid Crystal Society Award, Humboldt Award and many more.

19:30-20:00

Innovating Sustainable Catalyst Systems for Tackling CO_2 and H_2 Challenges

Sibudjing Kawi, National University of Singapore, Singapore

Sibudjing Kawi received his Bachelor, Master and PhD degrees from Univ. Texas, Univ. Illinois, and Univ. Delaware, respectively. After 2 year of postdoc at the Univ. California, he joined the Department of Chemical and Biomolecular Engineering, National University of Singapore in 1994. For more than a decade, his research focuses on catalysts and membranes for hydrogen production/separation and CO2 capture & utilization. He is a highly-cited researcher (2021, Clarivate). He has published > 330 journal papers (citations > 18,800, h index = 73), 5 patents, 1 book, 6 book chapters, edited > 12 special issues. He serves on the Editorial Board of 5 journals and Associate Editor of 2 journals. He is currently the lead PI for 3 projects (totaling > SGD 3 million) on CO2 capture/ utilization and H2 economy, as funded by NRF-NEA, A*STAR, and MOE.

20:00-20:30

Non-Thermal Plasma-Enhanced Catalysis-Decoupling Plasma-Induced Surface Reaction from Plasma-Phase Reaction

Chunshan Song, Chinese University of Hong Kong, Hong Kong

Chunshan Song is the Dean of Science and Professor of Chemistry at the Chinese University of Hong Kong and Distinguished Professor Emeritus at the Pennsylvania State University. His research focuses on chemistry and catalysis for energy and fuels including adsorptive CO_2 separation, catalytic CO_2 conversion, plasma catalysis, adsorptive and catalytic fuel processing, shape-selective catalysis and catalytic materials. He is a Fellow of American Chemical Society (ACS), has published 420 articles in refereed journals and received ACS George A. Olah Award, ACS Henry H. Storch Award, Herman Pines Award, Catalysis Club of Philadelphia Award, and Fulbright Distinguished Scholar Award.

Oral Presentations-II

Chair: Jim Jones, Massey University, New Zealand

20:30-20:50 **Global Catalysis Model for the Influence of Secondary Reactions on the Overall Heat of Pyrolysis of Biomass**
Jim Jones, Massey University, New Zealand

20:50-21:10 **Development of Heterogeneous Silver (I) Complex-Catalyst for Cyclization of Propargyl Amines with CO_2: Synthesis of Oxazolidinone Derivatives at Ambient Conditions**
Sangita Karanjit, Tokushima University, Japan

21:10-21:30 **Development of Catalysis Pathways in Regioselective C-H Activation**
Guanghui An, Heilongjiang University, China

21:30-21:50 **Direct Synthesis of Dimethyl Ether from CO_2 Hydrogenation over WOx-ZrO_2 Catalysts Admixed with a Cu-ZnO-ZrO_2 Catalyst**
Abrar Hussain, Yuan Ze University, Taiwan

21:50-22:10 **Cobalt Catalyzed C-H Functionalization**
Lukass Lukasevics, Latvian institute of Organic Synthesis, Latvia

Poster Presentations

22:10-22:15 **Immiscible Au-Pt Nanocatalyst for Direct Synthesis of Hydrogen Peroxide**
Geun-Ho Han, Korea University, South Korea

22:15-22:20 **Promoting Effect of Ligand Addition to the Activity of Hydrogen Peroxide Synthesizing Catalysts**
Seok-Ho Lee, Korea University, South Korea

End of Day-2

DAY 03

FEBRUARY 24, 2022

VIRTUAL | ROOM-1 & ROOM-2

PACIFIC TIME

Join the meeting
https://us02web.zoom.us/j/83449413825?pwd=dk5DQk9ibTFBczdvbjM2YWpvSFRxdz09
Meeting ID: 834 4941 3825
Passcode: 224460

Parallel Session-I

Materials

Mechanisms | Applications | Material Science | Zeolites | Polymers

Oral Presentations

Chair: Ravikrishnan Vinu, Indian Institute of Technology Madras, India

06:20-06:40 **Crystal Chemical and Topological Features of Microporous Beryllium Phosphate Zeolite-Type Materials**
Sergey M. Aksenov, Kola Science Centre, RAS, Russia

06:40-07:00 **Transitional Metal Complexes Based on nido-Carboranyl Amidines as a Potential Class of Novel Catalysts**
Marina Yu. Stogniy, Russian Academy of Sciences, Russia

07:00-07:20 **Human Peripheral Blood Mononuclear Cells Targeted Red-Light Emitting Switch for Selective Detection of HSO_3- Anion**
Sangita Das, Durham University, UK

07:20-07:40 **Obtaining Ultra-Thin Pan/Pitch-Based Fibers with Various Additivies by the Method of Electrospinning**
Zulkhair Mansurov, Al-Farabi Kazakh National University, Kazakhstan

07:40-08:00 **Platinum(IV) Complexes with Oxoanionic Ligands as Efficient Precursors for Catalytic Materials**
Danila B. Vasilchenko, Nikolaev Institute of Inorganic Chemistry, Russia

Poster Presentations

08:00-08:05 **Synthesis of Composite Carbon-Silicon Nanoparticles in a Gas-Phase Process**
Boris Ezdin, Novosibirsk State University, Russia

08:05-08:10 **Influence of Composition and Structural Characteristics on the Catalytic Properties of HZSM-5 Aluminosilicalites (MFI Type)**
Elena Domoroshchina, MIREA - Russian Technological University, Russia

Oral Presentations

08:10-08:30 **Tubular Photocatalytic Nanomaterials based on Wide-Band-Gap Compounds**
Ion Tiginyanu, Technical University of Moldova, Moldova

08:30-08:40 Break

Chair: Serena Esposito, Politecnico di Torino, Italy

08:40-09:00 **Implementation of Catalyst-Assisted Growth of III-V Semiconductors in HVPE Process**
Yamina Andre, Université Clermont Auvergne, France

09:00-09:20 **Role of Water in the Selective, Aerobic Oxidation of Methane over Pt-Based Catalysts**
Eric van Steen, University of Cape Town, South Africa

09:20-09:40 **What are the Oxidizing Intermediates in the Fenton and Fenton-Like Reactions?**
Dan Meyerstein, Ariel University, Israel

09:40-10:00 **Polydopamine Films from the Air/Water Interface and Their Photocatalytic Applications**
Emerson Coy, Adam Mickiewicz University, Poland

10:00-10:20 **Mg-Al Hydrotalcites as Catalysts of Baeyer-Villiger Oxidation of Cyclohexanone: The Effect of Precipitating Base and of Biopolymer Template**
Robert Karcz, Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Poland

10:20-10:40 **Assessing the Location and Nature of the Coke Formed in the Hydrocracking of a Refinery Refractory Stream**
Roberto Palos, University of the Basque Country, Brazil

10:40-11:00 **Sol-gel Approach for Active and Stable Silica Supported Ruthenium Catalysts for Hydrogenation Reactions**
Serena Esposito, Politecnico di Torino, Italy

11:00-11:20 Break

Chair: Marta Liras, IMDEA Energy, Spain

11:20-11:40 **Conjugated Porous Polymers: Ground-Breaking Materials for Solar Energy Conversion**
Marta Liras, IMDEA Energy, Spain

11:40-12:00 **Metal Oxides Nano-Size and Polymers Added MWCNTs for Hydrocarbons and Dyes Removal from Water**
Thamer Adnan Abdullah, University of Pannonia, Hungary

12:00-12:20 **Focused Ion Beam Time-of-Flight Secondary Ion Mass Spectrometry (FIB-TOF-SIMS) -A Powerful Technique for the Surface Characterization Taken to the Next Level by Fluorine Gas Coinjection**
Krzysztof Wieczerzak, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

12:20-12:40 **ZSM-5 Preparation from Waste: A Review**
Helena Schneider, Federal University of Rio Grande do Sul, Brazil

12:40-13:00 **Incorporation of Mo Into Husy Zeolite by Thermal Spreading and Evaluation of Ni Promoting Effect on Tetralin Hydroconversion Activity**
Bruno Martins Santos, PETROBRAS, Brazil

13:00-13:30 Break

Chair: Stewart P Lewis, Pyramid Polymers, Zanesville, OH

13:30-13:50 **Biopolymer Films and their Characteristics**
Sabine Gruener-Lempart, University of Applied Sciences Weihenstephan-Triesdorf, Germany

13:50-14:10 **Atomic/Nano-scale Surface and Interfacial Engineering for Fuel Cells and Electrolyzers**
Min Hwan Lee, University of California, Merced, CA

14:10-14:30	**Transforming Polymer Thermosets into Thermoplastics by Catalysis: Enhancing Sustainability via Dynamic Covalent Bonds and Tuning Dissociative vs. Associative Dynamic Chemistry, Reprocessability, and Elevated-Temperature Creep Resistance** **John M Torkelson**, Northwestern University, Evanston, IL
14:30-14:50	**Four Dimensional Acid Induced Polymerization of Olefins** **Stewart P Lewis**, Pyramid Polymers, Zanesville, OH
14:50-15:10	**X-Ray Atomic Imaging of Redox Induced Changes to Oxide Supported Catalysts** **Michael Bedzyk**, Northwestern University, Evanston, IL
15:10-15:30	**Dilute Alloy Catalysts Based on Au and Cu for Efficient Catalysis** **Juergen Biener**, Lawrence Livermore National Laboratory, Livermore, CA
15:30-15:50	**SMASH-ML: Automating the Synthetic Discovery of Nanomaterials** **Christopher Tassone**, SLAC National Accelerator Laboratory, Menlo Park, CA
15:50-16:10	Break
	Chair: Yuji Kikukawa, Kanazawa University, Japan
16:10-16:30	**Can the Indenyl Effect of Rh(III) Piano Stool Compexes Enhance Cyclometalation and Catalytic C–H Activation** **Joseph S. Merola**, Virginia Polytechnic Institute and State University, Blacksburg, VA
16:30-16:50	**Exploiting Automatic Image Processing and *in-situ* Transmission Electron Microscopy to Understand the Stability of Supported Nanoparticles** **Eric Stach**, University of Pennsylvania, Philadelphia, PA
16:50-17:10	**Modeling of Superacid Catalyzed Polyhydroxyalkylation of Modified Isatin and Biphenyl** **Eduardo Vivaldo-Lima**, Universidad Nacional Autónoma de México, Mexico
17:10-17:30	**Broadband Ultrafast Photoluminescence Spectroscopy and its Application in Material Characterization** **Kai Chen**, Victoria University of Wellington, New Zealand
17:30-17:50	**Kinetic Modeling of Nox Reduction Mechanism on TWC Catalysts by DFT Study** **Min Woo Lee**, Korea University, South Korea
17:50-18:10	**Synthesis and Catalysis of Nitrate-Incorporated Polyoxovanadates** **Yuji Kikukawa**, Kanazawa University, Japan
18:10-18:30	**Adsorption of Lactate and Ammonia by Layered Double Hydroxide and Zeolite** **Tomohito Kameda**, Tohoku University, Japan
18:30-18:40	Break
	Chair: Eduardo Vivaldo-Lima, Universidad Nacional Autónoma de México, Mexico
18:40-19:00	**Hard X-Ray Nanoprobe and Electrochemical Investigations of Ni-Co Based Materials for Supercapacitor** **Han-Wei Chang**, National United University, Taiwan
19:00-19:20	**Functional Oxides for High-performance Electrochemical Sulfur Cathodes** **Shen-Heng Chung**, National Cheng Kung University, Taiwan

19:20-19:40 **Preparation and Characterization of Mesoporous Zeolite Catalysts from Semiconductor/Optoelectronic Industries Flyashes for CO_2 Conversion into DME**
Ndumiso Vukile Mdlovu, Yuan Ze University, Taiwan

19:40-20:00 **Atomic-Design and Surface-Probing of Selective Two-Dimensional Nanomaterials as Artificial Leaves**
Li-Chyong Chen, National Taiwan University, Taiwan

20:00-20:20 **Synthesis of Single-Crystalline Transition Metal Dichalcogenide Thin Films Aiming for Catalyst Investigation**
Young Jun Chang, University of Seoul, South Korea

Poster Presentations

20:20-20:25 **p-Type to n-Type Conversion through the "Bypass" Structural Transformation in the Zintl Phase Thermoelectrics**
Tae-Soo You, Chungbuk National University, South Korea

20:25-20:30 **Two Steps to Improve the Thermoelectric Performance of the Ca_5−xYbxAl$_2$−yInySb$_6$ System**
Tae-Soo You, Chungbuk National University, South Korea

20:30-20:35 **p-Type Double Doping and the Diamond-like Morphology Shift of the Zintl Phase Thermoelectric Materials: The Ca11−xAxSb10−yGez (A = Na, Li; 0.06(3) ≤ x ≤ 0.17(5), 0.19(1) ≤ y ≤ 0.55(1), 0.13(1) ≤ z ≤ 0.22(1)) System**
Tae-Soo You, Chungbuk National University, South Korea

20:35-20:40 **Hydrothermal Synthesized Cobalt Catalyst with Enhanced Durability at High Temperature for CO and C_3H_6 Oxidation**
Haney Park, Korea University, South Korea

20:40-20:45 **The Mechanism of Pd in DSHP Reaction Through Halide Ion**
Seong-Yeon Hwang, Korea University, South Korea

20:45-20:50 **In situ TEM Investigation of Structural Changes in Ni Nanoparticle Catalysts under Methane Atmosphere**
Junko Matsuda, Kyushu University, Japan

PACIFIC TIME

Join the meeting
https://zoom.us/j/92295987408?pwd=aTJSQjMwcXZrUnRXbnRiR0RxYjNpZz09
Meeting ID: 922 9598 7408
Passcode: 420436

Parallel Session-II

Process-I

Electrocatalysis | Photocatalysis

Oral Presentations

Chair: Cornie VanSittert, North-West University, South Africa

06:40-07:00	**New Insights on Alcohols Electrooxidation in the Presence of Corresponding Aldehydes** **Ekaterina Zolotukhina**, Institute of Problems of Chemical Physics RAS, Russia
07:00-07:20	**Organically Modified Layered Perovskite-Like Oxides $HCa_2Nb_3O_{10}$, $HLnTiO_4$ and $H_2Ln_2Ti_3O_{10}$ (Ln = La, Nd) As Heterogeneous Photocatalysts for Hydrogen Production** **Oleg I. Silyukov**, Saint Petersburg State University, Russia
07:20-07:40	**DFT Investigation of Electrocatalyst delamination from Glassy Carbon Support** **Cornie VanSittert**, North-West University, South Africa
07:40-08:00	**Visible Photodegradation of Red Acid 1 Using Coal2o4@Cus as a Novel Photocatalyst** **Youssef Fahoul**, University of Sidi Mohamed Ben Abdellah, Morocco
08:00-08:20	**Organic-Inorganic Hybrid Photocatalytic Membranes for In-Flow Water Purification** **Ubirajara Pereira Rodrigues Filho**, University of São Paulo, Brazil
08:20-08:40	**Earth-Abundant Electrocatalyst for the OER within Zirconium Phosphate Nanoparticles** **Jorge L. Colón**, University of Puerto Rico, Puerto Rico
08:40-08:50	Break

Chair: Iryna Antonyshyn, Max Planck Institute for Chemical Physics of Solids, Germany

08:50-09:10	**TiO_2 and ZnO Containing Composite Nanofibers with High Photocatalytic Decomposition Performance Against Water Pollutants: Fabrication and Properties** **Mirela Suchea**, Hellenic Mediterranean University, Greece
09:10-09:30	**Modified Metal Oxide Nanostructures as Immobilized Photo-Catalysts for Degradation of Water Pollutant** **Andreja Gajovic**, Ruđer Boškovic Institute, Croatia
09:30-09:50	**Towards Suitable Solar Photocatalytic Wastewater-To-Hydrogen** **Alberto Puga**, Universitat Rovira i Virgili, Spain
09:50-10:10	**Structural, Morphological and Photocatalytic Behavior of Co-Doped ZnO** **Maria Eugenia Rabanal**, Carlos III University and IAAB, Spain

10:10-10:30 **Palladium Nanoparticles Hardwired in Carbon Nanoreactors Enable Continually Increasing Electrocatalytic Activity During the Hydrogen Evolution Reaction**
Maria del Carmen Giménez López, Universidade de Santiago de Compostela, Spain

10:30-10:50 **Controlling Factors on Electrochemical Determination of Flat Band Potential and Position of Band Edges of Titanium Dioxide**
Siaw Foon Lee, Institute of Construction Science "Eduardo Torroja", Spain

10:50-11:10 **Chemical Diversity of M_2Pt {M = Al, Ga, In, Sn} as OER Electrocatalysts**
Iryna Antonyshyn, Max Planck Institute for Chemical Physics of Solids, Germany

11:10-11:20	Break

Chair: Matthias Vandichel, University of Limerick, Ireland

Poster Presentations

11:20-11:25 **Synthesis and Characterization of Novel SBA-1 Mesoporous Silica Material Modified with Niobium**
Izabela Nowak, Adam Mickiewicz University, Poland

11:25-11:30 **Application of Biosilica Doped with Palladium Chloride Nanoparticles in the Photo catalytic Degradation of Methyl Orange**
Agnieszka Feliczak-Guzik, Adam Mickiewicz University, Poznań, Poland

11:30-11:35 **Fabrication of Photocatalysts by Laser Pyrolysis for Alkenes Production**
Juliette Karpiel, University of Paris-Saclay, France

Oral Presentations

11:35-11:55 **H-Graphdiyne/TiO_2 Heterojunction for Photocatalytic H_2 Generation**
Nawfal Ghazzal, Université Paris-Saclay, France

11:55-12:15 **Hydrothermal Treatment Assisted by Photocatalysis: An Innovative Process**
Chantal Guillard, CNRS-University of Lyon, France

12:15-12:35 **Protective Role of Sphingomyelin in Eye Lens Cell Membrane Model Against Oxidative Stress**
Christiane A. Helm, University of Greifswald, Germany

12:35-12:55 **Computational Electrochemistry Studies of OER and HER on Various Metal Systems**
Matthias Vandichel, University of Limerick, Ireland

12:55-13:15 **Tunability of ZnO Nanorods Properties Towards Enhanced Photocatalytic Performance**
Alejandro Galán-González, Durham University, UK

13:15-13:45	Break

13:45-14:05 **Electrodeposition of Nickel Hexacyanoferrate Film for Efficient Urea Oxidation Reaction**
Shun Lu, South Dakota State University, Brookings, SD

14:05-14:25 **Tuning the Properties of Metal Surfaces to make them CO-Tolerant and Highly Active Catalysts for Hydrogen Oxidation: A First-Principles Approach**
Sergey Stolbov, University of Central Florida, Orlando, FL

14:25-14:45	**Caustic Aqueous Phase Electrochemical Reforming (CAPER) for Process Intensified Compressed Hydrogen Production** **Su Ha**, Washington State University, Pullman, WA
14:45-15:05	**High Throughput Discovery of Oxygen Reduction Reaction Electrocatalysts** **John M Gregoire**, Caltech, Pasadena, CA
15:05-15:25	**Metamaterial Photocatalysis: An Archetype for Sustainable Chemical Fuels and Feedstock Industry** **Nazir Kherani**, University of Toronto, Canada
15:25-15:45	**Sodium Zinc Silicate as Green Photocatalyst for Transesterification Reaction Using Soybean Oil** **R. Rodríguez-Ramírez**, Unidad Profesional Interdisciplinaria en Ingeniería y Tecnologías Avanzadas, Mexico
15:45-16:05	**Rational Design of Photocatalysts for Sustainable Technologies** **Cameron Shearer**, The University of Adelaide, Australia
16:05-16:15	Break
	Chair: Tomoaki Takayama, Tokyo Institute of Technology, Japan
16:15-16:35	**3D Printing for Electrocatalysis** **Chong-Yong Lee**, University of Wollongong, Australia
16:35-16:55	**Photonic Crystal Enhanced Artificial Leaf with Non-Precious Metals for Water Splitting** **Qin Li**, Griffith University, Australia
16:55-17:15	**Nickel Hydroxides Derived from Nickel Dithiooxamide as Bifunctional Oxygen Electrocatalysts** **Izabela Rzeznicka**, Shibaura Institute of Technology, Japan
17:15-17:35	**DABCO-Promoted Electrochemical Dehydrogenative C–P Bond Formation Leading to Phosphacycles** **Koichi Mitsudo**, Okayama University, Japan
17:35-17:55	**Development of Plasmonic Photocatalysts** **Ewa Kowalska**, Hokkaido University, Japan
17:55-18:15	**Electrocatalytic CO_2 Reduction Over Noble-Metal Based Intermetallic Compounds in an Aqueous Solution** **Tomoaki Takayama**, Tokyo Institute of Technology, Japan
18:15-18:35	**Modification Strategies of TiO_2 Photocatalyst Coatings** **Sujun Guan**, Toyo University, Japan
18:35-18:45	Break
	Chair: Chung-Li Dong, Tamkang University, Taiwan
18:45-19:05	**Catalytic Application of Aluminum Doped Zinc Oxide Films Prepared by a Novel Mist Chemical Vapor Deposition Method** **Chaoyang Li**, Kochi University of Technology, Japan

19:05-19:25 **Solar-driven H_2O_2 Production by Nano Hybrid Photocatalysts and its Applications**
Hyoung-il Kim, Yonsei University, South Korea

19:25-19:45 **Effective Separation of Photogenerated Electron-Hole Pairs by Self-Doped Ti_3+ Black Anatase Tio_2−X Coupled with Cu Nanoparticles for Solar Energy Conversion**
Yeonho Kim, Incheon National University, South Korea

19:45-20:05 **Toward High-Performance and Stable Photoelectrochemical Water Splitting: Organic vs. Inorganic Photocatalyst**
Ji-Wook Jang, Ulsan National Institute of Science and Technology, South Korea

20:05-20:25 **TiO_2 Based Heterojunction Layers on IrO_2 Based Dimensionally Stable Anode for an Enhanced Reactive Chlorine Mediated Water Treatment**
Kangwoo Cho, Pohang University of Science and Technology, South Korea

20:25-20:45 **X-Ray Spectroscopic Investigation of Energy Materials**
Chung-Li Dong, Tamkang University, Taiwan

20:45-21:05 **Simple Modified Sol-Gel Synthesis of TiO_2 Photocatalysts for Glucose Conversion and Selectivity Changes in Production of Non-Caloric Sugars**
Surawut Chuangchote, King Mongkut's University of Technology Thonburi, Thailand

21:05-21:25 **Light Driven Ambient Temperature Conversion of Benzene to Phenol**
Joyeeta Lodh, Indian Institute of Science, Education and Research, India

End of Day-3

DAY 04

FEBRUARY 25, 2022

VIRTUAL | ROOM-1 & ROOM-2

PACIFIC TIME

Join the meeting
https://us02web.zoom.us/j/83449413825?pwd=dk5DQk9ibTFBczdvbjM2YWpvSFRxdz09
Meeting ID: 834 4941 3825
Passcode: 224460

Parallel Session-I

Energy

Energy Catalysis | Oil & Gas | Renewable Sources

Oral Presentations

Chair: Samuel Simon Araya, Aalborg University, Denmark

06:20-06:40 **Methyl Orange Application as a Mediator in Biofuel Cell with Anode based on *Escherichia coli***
Alisa S. Freiman, Institute of Problems of Chemical Physics RAS, Russia

06:40-07:00 **Carbon Supported Fe-K and Bimetallic Framework Catalysts for the CO Hydrogena tion into Olefins and Fuels**
Sergei Chernyak, Lomonosov Moscow State University, Russia

07:00-07:20 **Comparison of Biodiesel Synthesis by Oil Transesterification with Methanol and Butanol using Dolomite as a Heterogeneous Catalyst**
Ieva Gaide, Vytautas Magnus University, Lithuania

07:20-07:40 **Oxidation and Re-Carburisation of Potassium Promoted Fe-Based Fischer-Tropsch Catalysts Captured *in-situ***
Michael Claeys, University of Cape Town, South Africa

07:40-08:00 **Noble Metal Decorated $ZnBiVO_4$ Heterostructures for Enhanced Photocatalytic H_2 Production**
Katabathini Narasimharao, King Abdulaziz University, Saudi Arabia

08:00-08:20 **A New Technique for Preparation of Novel Sustainable Heterogeneous Polysaccha ride-Based Palladium Catalysts**
Oshrat levy-Ontman, Shamoon College of Engineering, Israel

08:20-08:40 **The Role of Hydrogen in the Green Transition via Power-to-X**
Samuel Simon Araya, Aalborg University, Denmark

08:40-08:50 Break

Chair: Anand Kumar, Qatar University, Qatar

08:50-09:10 **Surface Restricted Combustion Synthesis of NiCo/SiO_2 Catalysts for Methane Dry Reforming Reaction**
Anand Kumar, Qatar University, Qatar

09:10-09:30 **Reductive Activation of O_2 to O_{22}- from a Vanadium(IV) Species: Mechanism and Its Use in Fuel Cells**
Anastasios Keramidas, University of Cyprus, Cyprus

09:30-09:50 **Ion-Selective Electrocatalysis on Conducting Polymer Electrodes: Improving the Performance of Redox Flow Batteries**
Xavier Crispin, Linköping University, Sweden

Poster Presentations

09:50-09:55 **Molybdenum-Based Catalysts for Carbon Dioxide Conversion into Added-Value Products**
Daniel Deloglou, Aerosol and Particle Technology Laboratory/CERTH, Greece

09:55-10:00 **Study on Characteristics of CI Engine Supplied with Biodiesels from Brown and Yellow Greases**
Marek Wozniak, Lodz University of Technology, Poland

Oral Presentations

10:00-10:20 **Production of 5-Hydroxymethylfurfural from Apple Pomace in Deep Eutectic Solvent**
Katja Lappalainen, University of Oulu, Finland

10:20-10:30 Break

Chair: Stefano Falcinelli, University of Perugia, Italy

10:30-10:50 **Fuel Generation by Hydrogenation of Carbon Dioxide via Plasma-Assisted Catalysis**
Stefano Falcinelli, University of Perugia, Italy

10:50-11:10 **Homogeneous Catalysis for Low-temperature Biomass Valorization**
Martin Nielsen, Technical University of Denmark, Denmark

11:10-11:30 **Dual functional Materials Based on Ru or Ni on Alumina with Different Alkaline Metals for CO_2 Capture and Methanation**
Enrique Garcia Bordejé, Instituto de Carboquímica, Spain

11:30-11:50 **The Reaction Environment Controls the Steady State of Copper-Bearing Catalysts in Organosolv Lignin Fractionation**
Iqra Zubair Awan, ICGM Univ Montpellier, France

11:50-12:10 **Carbon Dioxide CO_2 as Feedstock for the Production of Chemical Intermediates**
Thomas Ernst Muller, Ruhr-Universität Bochum, Germany

12:10-12:30 **Smart Electrocatalytic {Mo-S}-Based Molecules for Hydrogen Generation**
Loic Assaud, University Paris Saclay, France

12:30-13:00 Break

Chair: Boniface Fokwa, The Regents of the University of California, Riverside, CA

13:00-13:20 **Binary SupraParticles for Heterogeneous Catalysis**
Alfons van Blaaderen, Utrecht University, The Netherlands

13:20-13:40 **Ternary Layered van der Waals Iron-based Chalcogenides for Efficient Hydrogen Evolution**
Boniface Fokwa, The Regents of the University of California, Riverside, CA

13:40-14:00 **Operating Parameter Effects on Mixed Alcohol Synthesis from Biomass Gasification**
Robert Cattolica, University of California, San Diego, CA

14:00-14:20	**Low-Temperature Photocatalytic Conversion of Natural Gas to Liquid Chemicals** **Yongchun Tang**, Power Environmental Energy Research Institute, Covina, CA
14:20-14:40	**Metal Phosphides: From Thermal Catalysis to Photocatalysis** **Mark Bussell**, Western Washington University, Bellingham, WA
14:40-15:00	**Hot Carrier-Driven Generation of Solar Fuels in Au/TiO_2 Nanoheterojunctions** **Karthik Shankar**, University of Alberta, Canada
15:00-15:20	**One-Step Upgrading of Real Flue Gas Streams to Low-Carbon Syngas over Alumina-Supported Catalysts** **Fabio Goncalves Macedo de Medeiros**, Université de Sherbrooke, Canada
15:20-15:30	Break
	Chair: Jochen Lauterbach, University of South Carolina, Columbia, SC
15:30-15:50	**Comparison of Experimental and Simulations Results of a Large-Scale Propane Jet Fire using CFD Method and PHAST Software: A Case Study** **Adriana Palacios Rosas**, Fundacion Universidad de las Americas, Mexico
15:50-16:10	**Biodiesel Production Catalyzed by Potassium Ferrate at Room Temperature** **Adriana N. Gutiérrez-López**, Instituto Politécnico Nacional, México
16:10-16:30	**Enabling Catalyst Discovery through High-Throughput Experimentation and Machine Learning** **Jochen Lauterbach**, University of South Carolina, Columbia, SC
16:30-16:50	**'Bubble-Free' Water Electrolysis that is Highly Energy Efficient** **Gerhard F. Swiegers**, University of Wollongong, Australia
16:50-17:10	**Low-Cost Catalysts for Next-Generation Fuel Cells** **Bram Hoex**, School of Photovoltaic and Renewable Energy Engineering, Australia
17:10-17:30	**Surface Atomic Structural Analysis of Nickel Plating Films Reacted with Methane at High Temperature Using HRTEM-EELS** **Kunichi Miyazawa**, Tokyo University of Science, Japan
17:30-17:50	**Electrochemical Utilization of Thylakoid Membranes and Cyanobacteria for the Solar Energy Conversion** **Sunghyun Kim**, Korea University, South Korea
17:50-18:10	**Sorbent for Concurrent Absorption of H_2S and COS in Coal-Derived Syngas** **Makoto Kobayashi**, Central Research Institute of Electric Power Industry, Japan
18:10-18:20	Break
	Chair: Sang-Chul Jung, Sunchon National University, South Korea
18:20-18:40	**Recent Advances in Hydrogen Production from Ammonia Decomposition** **Mostafa El-Shafie**, Gifu University, Japan
18:40-19:00	**CO_2-Free Hydrogen Production by Hydrothermal Cracking Using Liquid Phase Plasma from Hydrocarbons** **Sang-Chul Jung**, Sunchon National University, South Korea

19:00-19:20 **A study on the Optimization of Zr Loading Amount of Co-Zr-CeO_2 Catalyst for High Temperature Shift Reaction**
Tae-Yeol Choi, Changwon National University, South Korea

19:20-19:40 **Potential Reductions in Global Gas Flaring for Determining the Optimal Sizing of Gas-To-Wire (GTW) Process: An Inverse DEA Approach**
Kelvin K. Orisaremi, The Hong Kong Polytechnic University, Hong Kong

19:40-20:00 **Facile One-Pot Synthesis of Nimos/SBA-15 Catalysts for Hydrodesulfurization**
Antony Rajendran, Taiyuan University of Technology, China

20:00-20:20 **Liquefaction of Waste Tire Rubber Chips for Absorptive Recycling of Spilled Oils**
Cerelia Danica Samora Aberdeen, Yuan Ze University, Taiwan

20:20-20:40 **Hydrodeoxygenation of Model Biomass Oxygenate Mixtures: Evidence of Cross-reactivity over Pt/HY Catalyst**
Vallabh Prabhudesai, Indian Institute of Technology Madras, India

20:40-21:00 **Influence of Surface Properties of Ag Nanocomposites Resulting from Green Synthesis on the Antibacterial Activity**
Beata Lesiak-Orłowska, Polish Academy of Sciences, Poland

Poster Presentations

21:00-21:05 **Effect of Precipitant in the Production of Cu/CeO_2 Catalyst for Water Gas Shift Reaction**
Yong-Hee Lee, Changwon National University, South Korea

21:05-21:10 **Ni-$CeZrO_2$ Catalyst Performance Evaluation According to Promoter (Mgo, La_2O_3, Cao) in Biogas Steam Reforming Reaction**
Yu-Seung Heo, Changwon National University, South Korea

21:10-21:15 **Ni-Ce Based Mixed Oxide Catalysts with Perovskite Structure for the Biogas Steam Reforming**
Min-Ju Park, Changwon National University, South Korea

21:15-21:20 **A Study on the Promoted Ni-CeO_2 Catalysts for the High Temperature Water Gas Shift Reaction to Produce Hydrogen from Waste Derived Synthesis Gas**
Hak-Min Kim, Changwon National University, South Korea

PACIFIC TIME

Join the meeting
https://zoom.us/j/92295987408?pwd=aTJSQjMwcXZrUnRXbnRiR0RxYjNpZz09
Meeting ID: 922 9598 7408
Passcode: 420436

Parallel Session-II

Process-II

Environmental Catalysis | Industrial Catalysis | Nanocatalysis

Oral Presentations

Chair: Herman S. Mansur, Universidade Federal de Minas Gerais, Brazil

07:00-07:20	**A Non-Enzymatic Glucose Sensor based on *Limonia acidissima* Groff Tree Extract Gum Decorated Palladium Nanoparticles** **Kondaiah Seku**, University of Technology and Applied Sciences, Oman
07:20-07:40	**Hierarchical Zeolites as Catalysts for Biodiesel Production from Waste Frying Oils to Overcome Mass Transfer Limitations and Assess the Influence of Si/Al Ratio** **Elyssa Fawaz**, American University of Beirut, Lebanon
07:40-08:00	**Badler-Dauben and Isomerization Reactions of Allylic Alcohols in Acid-Water Media Catalyzed by Surfactant-Stabilized Colloidal Palladium Nanoparticles** **Brunno Lange Albuquerque**, Federal University of Rio Grande do Sul, Brazil
08:00-08:20	**The Role of Cobalt Doping Content on the Catalytic Activity of Iron Oxide-Carboxymethylcellulose Hybrid Magnetic Nanocatalysts for Organic Pollutant Degradation in Aqueous Phase** **Herman S. Mansur**, Universidade Federal de Minas Gerais, Brazil
08:20-08:40	**Effect of Nanoparticle Size in Pt/Al_2O_3 Catalyzed Sulfate Reduction in Liquid Phase** **Satu Pitkaaho**, University of Oulu, Finland
08:40-09:00	**Highly Efficient Antimicrobial Catalysts** **Yiping Zhao**, University of Georgia, Athens, GA
09:00-09:20	**Advanced Biofuels Towards a Carbon Neutral Economy** **Stella Bezergianni**, CERTH, Greece
09:20-09:40	**Protic Ionic Liquids from Di- or Triamines: Even Cheaper, Reusable Catalysts for Brønsted Acid-Mediated Transformations** **Alina Brzeczek-Szafran**, Silesian University of Technology, Poland
09:40-09:50	Break

Chair: Ian Shuttleworth, Nottingham Trent University, UK

09:50-10:10	**Nickel Nanowires Decorated by Palladium as a Novel And Efficient Catalyst for Ethanol Oxidation Reaction in Alkaline Medium** **Dariusz Lukowiec**, Silesian University of Technology, Poland
10:10-10:30	**Interparticle Reactions: A new form of Nanochemistry** **Krishnadas Kumaranchira Ramankutty**, University of Geneva, Switzerland

10:30-10:50 **Catalysts from Non-Critical Raw Material for Sustainable Chemistry**
Lucia D'Accolti, University of Bari Aldo Moro, Italy

10:50-11:10 **Synthesis of Metallic Nanoparticles for Heterogeneous Catalysis : Application to the Direct Borohydride Fuel Cell**
Thomas Maurer, Université de Technologie de Troyes, France

11:10-11:30 **Use of Nanostructured Catalyst for Green Chemistry Applications**
Antonio Monopoli, University of Bari Aldo Moro, Italy

11:30-11:50 **Green Chemistry and Catalysis the Way Forward**
Walter Cabri, University of Bologna, Italy

11:50-12:10 **Dehydrogenation of Formic Acid Attained by Highly Stable Catalysts Derived from Soft-Biomass Residues**
Miriam Navlani Garcia, Universidad de Alicante, Spain

12:10-12:30 **How Long is a Piece of String?**
Ian Shuttleworth, Nottingham Trent University, UK

12:30-13:00 Break

Chair: Yujun Shi, University of Calgary, Canada

13:00-13:20 **Disinfection By-Products from UV-LED/Chlorine Treatment**
Irene Carra, Cranfield University, UK

13:20-13:40 **Surface Chemistry of Graphene on Ruthenium and Pt/Graphene on Ruthenium–Adsorption and Reaction of SO_2, H_2S, and CO**
Uwe Burghaus, North Dakota State University, Fargo, ND

13:40-14:00 **Importance of Research Advancements in the Refining Industry**
Melissa Clough Mastry, BASF Corporation, Iselin, NJ

14:00-14:20 **Trials and Tribulations in Oxidative Coupling of Methane**
David West, SABIC Technology and Innovation, Sugar Land, TX

14:20-14:40 **New Insights in Constructing an Efficient Cu Catalyst for CO And NO Removal**
Fudong Liu, University of Central Florida, Orlando, FL

14:40-15:00 **New Perspectives and Insights into Silver Catalyzed Direct Propylene Epoxidation**
Anne M. Gaffney, University of South Carolina, Columbia, SC

15:00-15:20 **Carbon Nanotube Synthesis from FC-CVD Method using in-situ Delivery of Ferrocene Powder**
Devika Chauhan, University of Cincinnati, Cincinnati, OH

15:20-15:40 **Au-catalyzed Growth of β-Ga_2O_3 Nanowires**
Yujun Shi, University of Calgary, Canada

15:40-15:50 Break

Chair: Keiko Waki, Tokyo Institute of Technology, Japan

15:50-16:10 **Synthesis and Catalytic Activity of 2M WS_2 for Water Splitting Reactions**
Brian Leonard, University of Wyoming, Laramie, WY

16:10-16:30 **Cu/Al_2O_3 Catalyzes photo-Fenton to Remove Bisphenols**
Reyna Natividad, Universidad Autónoma del Estado de México, Mexico

16:30-16:50 **Three-Way Catalytic Performance and Microstructure of M-Al_2O_3 (M = Fe, Mn) Supported Pt Catalysts**
Masatomo Hattori, Nagoya University, Japan

16:50-17:10 **Efficient Ru/CeO_2/MgO Catalysts for CO_2-Free Green Ammonia Synthesis**
Rahat Javaid, National Institute of Advanced Industrial Science and Technology, Japan

17:10-17:30 **Design and Synthesis of Metallosupramolecular Phosphatases Functionalized with Lewis Acidic Sites by the Self-Assembly of Molecular Building Blocks**
Shin Aoki, Tokyo University of Science, Japan

17:30-17:50 **Catalytic Activity Derived from the Defective Structures of Carbon Nanotubes for Oxygen Reduction Reaction**
Keiko Waki, Tokyo Institute of Technology, Japan

17:50-18:10 **Hollow Nanoreactors for Bioorthogonal Catalysis in Living Systems**
In Su Lee, Pohang University of Science and Technology, South Korea

18:10-18:20 Break

Chair: Satoshi Kaneko, Tokyo Institute of Technology, Japan

18:20-18:40 **Theoretical Study on the Dry Reforming of Methane**
Yoshitada Morikawa, Osaka University, Japan

18:40-19:00 **The Formation of Dense α-Fe_2O_3 Nanostructures by Thermal Oxidation of Iron in Water Vapor and Its Capability on Cr(VI) Adsorption**
Faisal Budiman, Telkom University, Indonesia

19:00-19:20 **Photo-oxidation and Reaction Kinetics of Hg0 by Using CeO_2/TiO_2{101} and {001} at High Temperatures in the Atmosphere of Air Pollutants**
Chung-Shin Yuan, National Sun Yat-sen University, Taiwan

19:20-19:40 **Electrochemical Valorization of Biodiesel Waste for Biodegradable Plastic Precursor Production**
Jason Lam, City University of Hong Kong, Hong Kong

19:40-20:00 **Preparation and Characterization of Biochar-supported nZVI Nanocomposites from Rice Husks for Nitrophenol Wastewater Degradation**
You-Sheng Lin, Yuan Ze University, Taiwan

20:00-20:20 **Sonophotocatalytic Mineralisation of Antibiotics Using N-TiO_2 Catalyst: Process Optimisation, Mechanism and Degradation Intermediates**
Amritanshu Shriwastav, Indian Institute of Technology Bombay, India

20:20-20:40 **Vibrational Spectroscopy for Detection of Localized Surface Plasmon-Induced Reaction on a Single-Molecule Scale**
Satoshi Kaneko, Tokyo Institute of Technology, Japan

Poster Presentations

20:40-20:45 **Effect of Alkalis on Precipitated Iron-Based Catalysts for High-Temperature Fischer-Tropsch Synthesis**
Yi Yang, East China University of Science and Technology, China

20:45-20:50 **Simultaneous Removal of Particulates and NO over Tice0.25Sn0.25Ox/P84 Catalytic Filters from Flue Gas**
Maoseng Ni, Nanjing University of Information Science & Technology, China

End of Day-4

DAY 05

FEBRUARY 26, 2022

VIRTUAL | ROOM-1

PACIFIC TIME

Join the meeting
https://us02web.zoom.us/j/83449413825?pwd=dk5DQk9ibTFBczdvbjM2YWpvSFRxdz09
Meeting ID: 834 4941 3825
Passcode: 224460

Chemical Engineering

Organometallics Chemistry | Physical Chemistry | Quantum Chemistry | Reaction Engineering | Simulation & Modeling

Oral Presentations

Chair: Mirosław Szukiewicz, Rzeszow University of Technology, Poland

07:00-07:20	**Subtle Features in Lactide Polymerization: Effect of Metal, Ligand(s) and Geometry of Catalyst in PLA Synthesis** **Debashis Chakraborty**, Indian Institute of Technology Madras, India
07:20-07:40	**Understanding the Different Effects of Lanthanide and Alkali Promoters on Cobalt Catalyzed Fischer-Tropsch Synthesis: Insights from Molecular Modelling** **Ali Can Kizilkaya**, Izmir Institute of Technology, Turkey
07:40-08:00	**Catalytic Oxidative Degradation of Cresol Isomers Using Mn, Fe, and Ni Supported V_2O** **Rajasekhar VSR Pullabhotla**, University of Zululand, South Africa
08:00-08:20	**The Moment Equations for Catalytic Fixed Bed Reactor** **Mirosław Szukiewicz**, Rzeszow University of Technology, Poland
08:20-08:40	**Heck Coupling Reactions Catalyzed by Pd Nanoparticles in the Presence of an Ionic Liquid** **Agnes Mastalir**, University of Szeged, Hungary
08:40-09:00	**Optical Anisotropy Evolution of Thin Porphyrin Films Grown on HOPG During the Molecular Oxidation in Acid Electrolytes** **Gianlorenzo Bussetti**, Politecnico di Milano, Italy
09:00-09:20	**Quantum Chemical Design of Heterogenous Electrocatalysts for the Nitrogen Reduction Reaction that are Synthetically Feasible** **Tore Brinck**, KTH Royal Institute of Technology, Sweden
09:20-09:40	**Quantum Chemical Assessment of Well-Defined Catalysts for the Oxygen Reduction Reaction** **Christopher Ehlert**, Heidelberg Institute for Theoretical Studies, Germany
09:40-09:50	Break

Chair: Mehrdad Nikavech, University Sorbonne Paris Nord, France

09:50-10:10	**Up-Grading of Syngas Quality by a Coupled Thermal and Catalytic Tar Cracking** **Maria Laura Mastellone**, Università Vanvitelli, Italy
10:10-10:30	**Mechanism of Producing Metallic Nanoparticles, with an Emphasis on Silver and Gold Nanoparticles, Using Bottom-Up Methods** **Haya Kornweitz**, Ariel University, Israel

10:30-10:50	**Noncovalent Interactions, a New Perspective for a Rational Engineering in Homogenous Catalysis?** **Jean-Pierre Djukic**, Strasbourg University, France
10:50-11:10	**Growth Mechanisms of Carbon Nanotubes on Small Metallic Catalysts by Chemical Vapor Deposition** **Yann Magnin**, MIT/TOTAL/SEAOWL, France
11:10-11:30	**Effects of TiO_2 Stoichiometry and Oxygen Defects in the Photocatalytic Degradation of Cefexim Under Solar and Artificial Light Illuminations** **Fatemehsadat MOOSAVI**, University Sorbonne Paris Nord, France
11:30-11:50	**Copper Catalyzed Addition of Grignard Reagents to M.A., A Computational Perspective** **Marta Castineira Reis**, Universidade de Santiago de Compostela, Spain
11:50-12:10	**Iron-Catalyzed Enantioselective Intramolecular Inverse Electron-Demand HDA Reactions** **Jean-Marc Campagne**, ENSCM, France
12:10-12:30	**Babler-Dauben and Isomerization Reactions** **Brunno Lange Albuquerque**, Universidade Federal do Rio Grande do Sul, Brazil
12:30-13:00	Break
	Chair: Robert Walker, Montana State University, Bozeman, MT
13:00-13:20	**Olefin Metathesis Catalyzed by Vanadium Complexes** **Konstantin Bukhryakov**, Florida International University, Miami, FL
13:20-13:40	**Platinum-Catalyzed C-H Acylation of 2-Aryloxypyridines: Scope, Limitations, and Mechanistic Aspects** **Shouquan Huo**, East Carolina University, Greenville, NC
13:40-14:00	**HGM Concept for Non-Oxidative Dehydrogenation - 10 Years of the Commercial Experience** **Vladimir Fridman**, Clariant Corporation, Louisville, KY
14:00-14:20	**Operando Optical Studies of High Temperature Electrochemical Oxidation and Carbon Remediation** **Robert Walker**, Montana State University, Bozeman, MT
14:20-14:40	**In Operando Molecular Imaging of the Electrode and Liquid Electrolyte Interface** **Xiao-Ying Yu**, Pacific Northwest National Laboratory, Richland, WA
14:40-15:00	**Effects of Enzyme-Ligand Interactions on the Photoisomerization of a Light-Regulated Chemotherapeutic Drug** **Ruibin Liang**, Texas Tech University, Lubbock, TX
15:00-15:20	**Exploring Catalysis with Quantum Chemistry and Machine Learning** **Konstantinos Vogiatzis**, University of Tennessee, Knoxville, TN
15:20-15:30	Break

Chair: Adriana Palacios Rosas, Fundacion Universidad de las Americas, Mexico

15:30-15:50 **Ultrafast Dynamics of Hot Electron-driven Photocatalysis in Plasmon-Resonant Grating Structures**
Stephen Cronin, University of Southern California, Los Angeles, CA

15:50-16:10 **Dynamics Effects in Metal Catalyzed Allylic Bond Activation**
Lawrence M Wolf, University of Massachusetts, Lowell, MA

16:10-16:30 **Rational Design of High Entropy Alloys for Electrocatalysis Applications**
Luis Ruiz Pestana, University of Miami, Coral Gables, FL

16:30-16:50 **Correlating FEM, BEM and DDA Methodologies for Quantitative Analysis of Electron-Matter and Light-Matter Interactions in Metal Oxide Assemblies**
Progna Banerjee, The University of Texas at Austin, Austin, TX

16:50-17:10 **Probing Complex Interfaces Using Ab-Initio Simulations and Experimental Characterizations**
Tadashi Ogitsu, Lawrence Livermore National Laboratory, Livermore, CA

17:10-17:30 **Semicontinuum (Cluster-Continuum) Modeling of Acid-Catalyzed Aqueous Reactions: Alkene Hydration**
Allan East, University of Regina, Canada

Poster Presentations

17:30-17:35 **Synthesis and Application of Heteroaryl 1,2-Diketones via Palladium Catalysis**
Lili Ma, Northern Kentucky University, Highland Heights, KY

17:35-17:40 **Development of Core-Shell Catalysts for Fischer-Tropsch Synthesis in 3D Printed SS Microchannel Microreactors**
Meric Arslan, North Carolina A&T State University, Greensboro, NC

17:40-17:50 Break

Oral Presentations

Chair: Konstantinos Vogiatzis, University of Tennessee, Knoxville, TN

17:50-18:10 **Boron Group Doping to Adjust Electronic Structure of 2D $Mg(OH)_2$ for Visible-Light Photocatalytic Applications**
Shunnian Wu, Singapore University of Technology and Design, Singapore

18:10-18:30 **Unstable Intermediates for CO_2 Conversion into Methanol on a Cu(111) Model Catalyst**
Kotaro Takeyasu, University of Tsukuba, Japan

18:30-18:50 **Computation-Aided Catalyst Screening for Efficient Ammonia Synthesis**
Qinghong Yuan, East China Normal University, China

18:50-19:10 **Electronically Tuned Meso-Phenyl Substituted Vanadium Porphyrins: Synthesis, Characterization, and Catalytic Application in Selective Epoxidation of Olefins**
Chanchal Haldar, Indian Institute of Technology, India

19:10-19:30 **Synthesis and Characterization of Palladium Nanocrystals-Nitrogen Doped Carbon Dots: Heck Reaction**
Muhammad Sadiq, University of Malakand, Pakistan

Poster Presentation

19:30-19:35 **Oxidative Coupling of Methane Over Alkaline-Earth Metal Oxide-Promoted Lanthanum-Oxide Catalysts**
Anusorn Seubsai, Kasetsart University, Thailand

End of Day-5

PROGRAM

We wish to see you at

CCE-2023

Las Vegas, NV

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