IV International Conference on
Catalysis and Chemical Engineering
February 24–26
2020

Venue
Four Points by Sheraton
Los Angeles International Airport
9750 Airport Boulevard
Los Angeles, CA 90045, United States

The event invitation code is: cathv

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Day 1

07:20-08:00 Registrations and Badge Pickup
08:00-08:10 Opening Ceremony by Mannar Ram Maurya, Dean of Indian Institute of Technology Roorkee, India

Introductory Lecture @ California BallRoom A&D

Mannar Ram Maurya
Indian Institute of Technology Roorkee, India

Title: Catalytic Potentials of Polymer Supported Metal Complexes

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 and Assistant Professor from 1996-2008 and as a Professor in I.I.T. Roorkee from 2008-till now. He carried out many projects associated with vanadium and molybdenum chemistry. Major emphases were on the synthesis of vanadium complexes, their encapsulation in the cavity of zeolite-Y and immobilization on organicpolymers and their uses as recyclable and sustainable systems for catalytic oxidation of organic substrates. Effort was also made to identify the intermediate(s) to understand the mechanism of the catalytic reactions. He worked as a Guest Editor for Topics in Catalysis and Catalysis Today for Special Issues published based on the papers presented in 2nd and 3rd International Conference on Catalysis and Chemical Engineering, respectively.

Plenary Presentations @ California BallRoom A&D

Gabor A. Somorjai
University of California, Berkeley, CA

Title: Integrating the Three Fieldes of Catalysis: Active Site Engineering in Metal Nanoparticles/Cluster/Single

Gabor A. Somorjai is currently University Professor at University of California, Berkeley, CA. Concurrent with his faculty appointment, he is also a Faculty Senior Scientist in the Materials Sciences Division, and Group Leader of the Surface Science and Catalysis Program at the Center for Advanced Materials, at the E.O. Lawrence Berkeley National Laboratory. He educated more than 130 Ph.D. students and 250 postdoctoral fellows. He is the author of more than 1200 scientific papers in the fields of surface chemistry, heterogeneous catalysis, and solid state chemistry. He has written four textbooks, Principles of Surface Chemistry, Prentice Hall, 1972; Chemistry in Two Dimensions: Surfaces, Cornell University Press, 1981; and Introduction to Surface Chemistry and Catalysis, Wiley-Interscience, 1994 and the Second Edition in 2010; as well as a monograph, Adsorbed Monolayers on Solid Surfaces, Springer-Verlag, 1979. He is known as the Father of Modern Surface Chemistry. He received many awards including Wolf Prize in chemistry in 1998, National Medal of Science in 2002, Priestley Medal in 2008 and many more. He is also a member of National Academy of Sciences, Hungarian Academy of Science, Chemical Society of Japan.
Title: New Quantum Mechanics Based Methods for Multiscale Simulations of Catalysis with Focus on Reaction

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 systems and is actively involved in applying these methods to ceramics, semiconductors, superconductors, thermoelectrics, metal alloys, polymers, proteins, nuclei acids, Pharma ligands, nanotechnology, and energetic materials. He is a member of the International Academy of Quantum Molecular Science and the U.S. National Academy of Sciences. He has published 1363 articles with an H index = 156, I-10 index 1191. He received many notable awards including NASA Space Sciences Award for Space Shuttle Sensor (2009), polymer films (2012), ISI Highly Cited Chemist for 1981–2001, 2014, 2015, 2016, Named Clarivate Analytics Highly Cited Researcher 2018 and 2019.

Title: Photocatalytic Conversion of Nitrogen to Ammonia

Jimmy C Yu is Choh-Ming Li Professor of Chemistry and Head of United College at The Chinese University of Hong Kong. He is also an Associate Director of Institute of Environment, Energy and Sustainability, CUHK. Prof. Yu is a founding member of the first environmental science program in Hong Kong. His major research interest is photocatalysis, and he holds several patents on photocatalytic nanomaterials. Prof. Yu is a Clarivate Analytics Highly Cited Researcher (Cross-Field). He has received many honors including a State Natural Science Award and Chang Jiang Scholar Chair Professorship.

Title: Polyoxometalate Catalysts in Solar Fuels and Cancer Chemotherapy

Craig L. Hill Goodrich White Professor at Emory University, has been studying catalysis, reaction mechanisms and materials science for many years. Current research focuses on solar fuels, catalytic and multi–electron transfer processes, frequently with an emphasis on nano-scale materials and POM derivatives. He has trained ~140 graduate students and postdocs. Google Scholar lists ~410 publications cited ~28,000 times (H index = 90) with four cited over 1000 times. He has received three ACS awards, many others and is a Fellow of AAAS, the Victorian Institute of Chemical Sciences, the Academia Europaea, and the Royal Society of Chemistry. He is Nominator for 1992–present Nobel Prizes in Chemistry (1992–present).
Keynote Presentations

**Witko Malgorzata**
Jerzy Haber Institute of Catalysis and Surface Chemistry Polish Academy of Sciences, Poland  
11:40–12:10

**Title:** Catalytic Activity of Selected Heteropolyacids as a Function of their Chemical Composition: Theory versus Experiment

Małgorzata Witko currently Director of Institute of Catalysis and Surface Chemistry, PAS, Her research topics mainly on Model theoretical studies in the field of heterogeneous, homogeneous, and enzymatic catalysis focusing on the studies of electronic (influence of a support and additives, ligand) and steric (mutual orientation of reagents) effects determining selectivity and reactivity in catalytic reactions. She is acting as a Vice President of EFCACT (European Federation on Catalysis) and Vice President of Committee of Chemistry, Polish Academy of Sciences. She received award of the President of Polish Academy of Sciences in 1978.

**Francisco Zaera**
University of California, Riverside, CA  
12:10–12:40

**Title:** New Nanostructures for Increased Selectivity and Stability in Catalysis

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. His research interests are in surface and materials chemistry and in heterogeneous catalysis.

**Zhifeng Ren**
University of Houston, Houston, TX  
13:50–14:20

**Title:** Hydrogen Production from Water Splitting by Electrolysis

Zhifeng Ren is currently the M.D. Anderson Chair Professor in the Department of Physics and TcSUH of the University of Houston. He obtained Ph.D. degree from the Institute of Physics Chinese Academy of Sciences in 1990, specializes in materials synthesis and applications, especially in nanostructured thermoelectric materials, devices, and systems for more efficient energy conversion using the enhanced thermoelectric materials. He was an Outstanding Overseas Chinese Young Investigator, Nanjing University, China, 2005, Distinguished Senior Research Award, Boston College, 2006, received R&D 100 Award for the Development of High Performance Thermoelectric Materials, 2008, He Ranked as the 49th of the World's Top 100 Materials Scientists of the Decade (2000–2010), 2011. He is Editor-in-Chief of Materials Today Physics and many more journals. He was a co-founder of NanoLab, Inc., 2000, Commercialization of Carbon Nanotubes, Solasta, Inc., 2006. He worked as a Board of Directors, GMZ Energy China, 2011–2015.
Debbie C. Crans
Colorado State University, Fort Collins, CO

**Title:** Selective Interaction of Vanadium(IV) Coordination Complexes with Plasma Membrane Lipids Leading to G Protein-Coupled Receptor Signal

Debbie C. Crans is a professor of chemistry at Colorado State University, Fort Collins, CO. Her research interests include 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.

Gregory S. Herman
Oregon State University, Corvallis, OR

**Title:** Oxidation of Isopropyl Alcohol by SnO$_2$ (110)

Gregory S. Herman received his B.S. degree in Chemistry at the University of Wisconsin-Parkside in 1985 and his PhD. in Physical Chemistry at the University of Hawaii at Manoa in 1992. In 1992 Gregory received a National Research Council Postdoctoral Fellowship at the Naval Research Laboratory and performed research at the National Synchrotron Light Source at Brookhaven National Laboratory. Later in 1992 he began a second postdoctoral fellowship at Pacific Northwest National Laboratory (PNNL). From 1995 until 2000 Gregory was a senior research scientist in the Environmental Molecular Sciences Laboratory at PNNL. From 2001 until 2007 he was an R&D engineer in the Advanced Materials and Processes Laboratory at Hewlett-Packard Corporation. From 2007 until 2009 he was a senior scientist in the Materials and Device Applications Laboratory at Sharp Laboratories of America. In 2009 he joined the School of Chemical, Biological and Environmental Engineering at Oregon State University (OSU) as an associate professor and was promoted to professor in 2015. In 2019, he was appointed head of the school and named the James and Shirley Kuse Chair in Chemical Engineering.

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

**Title:** Computational Chemistry Methodologies for Transition Metals and Beyond

Angela K. Wilson is a computational, theoretical, and physical chemist. She is the John A. Hannah Distinguished Professor of Chemistry and the Associate Dean for Strategic Initiatives in the College of Natural Sciences at Michigan State University. She also serves as the Director of the MSU Center for Quantum Computing, Science, and Energy (MSU-Q). She has served as Division Director (head) of the Division of Chemistry at the U.S. National Science Foundation. Among her recognitions are Fellow of the American Chemical Society, American Physical Society, and the American Association for the Advancement of Science (AAAS), and the Francis P. Garvan–John M. Olin Medal. She is currently Chair of the Chemistry Section of AAAS, and is a nominee for President of the American Chemical Society.
Debasish Kuila  
National University of Singapore, Singapore

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<td>16:10-16:40</td>
<td>Debasish Kuila</td>
<td><strong>Title</strong>: Fischer-Tropsch Studies in 3-D Printed SS Microreactors: Effect of Mesoporous Silica, 2nd Metal and Mesoporous Composite Oxide Support&lt;br&gt;&lt;br&gt;Debasish Kuila, previous Chair and Professor of chemistry, is the Research Director of NSF- CREST Bioenergy Center at North Carolina A&amp;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.</td>
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Sibudjing Kawi  
National University of Singapore, Singapore

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<td>16:40-17:10</td>
<td>Sibudjing Kawi</td>
<td><strong>Title</strong>: Strategies to Develop Efficient Catalytic Systems for CO₂ Utilizations&lt;br&gt;&lt;br&gt;Sibudjing Kawi is currently with the Department of Chemical and Biomolecular Engineering, National University of Singapore. He received MSc (Chem. Eng.) from Illinois in 1988 and BSc (Chem. Eng) from Texas in 1985. He obtained PhD in Chemical Engineering from Delaware in 1992. His research interests include studies on next generation catalyst that will provide a knowledge base for novel synthesis techniques and molecular engineering of highly active and selective catalysts, as well as the design and growth of novel inorganic membranes preferred by industries.</td>
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Cat P-01  Use of Nb$_2$O$_5$,$n$H$_2$O and Nb$_2$O$_5$/Al$_2$O$_3$ as Acids Catalysts for the Dehydration of Xylose to Furfural  
Leticia Franzo de Lima, University of Campinas, Brazil

Cat P-02  Facile Synthesis and Characterization of Ag(NP)/TiO$_2$ Nanocomposite: Photocatalytic Efficiency of Catalyst for Oxidative Removal of Alizarin Yellow  
Seung-Mok Lee, Catholic Kwandong University, South Korea

Cat P-03  Preparation and Characterization of Ni/Al$_2$O$_3$ for Carbon Nanofiber Production from CO$_2$ Hydrogenation  
You-Sheng Lin, Yuan Ze University, Taiwan

Cat P-04  Pt$_x$-(H$_x$MoO$_3$)$_y$ CO-Tolerant Anode Catalysts for PEMFCs  
Kirill Kurdin, Skolkovo Institute of Science and Technology, Russia

Cat P-05  Preparation and Characterization of Amorphous Binary Catalysts in Alkaline Solutions for Hydrogen Evolution Reaction  
Kirill Kurdin, Skolkovo Institute of Science and Technology, Russia

Cat P-06  A Comparative Study of Support Oxide Over Ni Based Catalysts for Dry Reforming of Methane  
Ju–Hwan Kim, Changwon National University, South Korea

Cat P-07  The Comparison of Cu/CeO$_2$ Catalyst Using Different Precipitants for Low Temperature Water Gas Shift Reaction  
Yun–Jung Gu, Changwon National University, South Korea

Cat P-08  The Effect of Cu Loading on Co-Precipitated Cu–CeO$_2$ Catalyst for LT-WGS Reaction  
Hui–Ju Byeon, Changwon National University, South Korea

Cat P-09  Study of a Novelty Hydroxyapatite/g–C$_3$N$_4$ Hybrid Material as a High Performance Photocatalyst  
Angeles Mantilla, Instituto Politécnico Nacional, Mexico

Cat P-10  The Comparison of Catalytic Performance According to Preparation Method of Fe–Al–Cu Catalyst for HT-WGS Reaction  
Chang–Hoon Jeong, Changwon National University, South Korea

Cat P-11  Analysis of Battery Storage System Characteristics in Residential Building  
Peter Virtic, University of Maribor, Slovenia

Cat P-12  Integration of Biobased Material in Heterogeneous Catalysts Design for Energy and Circular Economy Application  
Sana LABIDI, Strasbourg University, France

Cat P-13  Elucidation of the Formation of the Carbon Microcoils Using Different-Sized Ni Catalysts  
Sung–Hoon Kim, Silla University, South Korea

Cat P-14  Cis–labile Iron NHC Complexes in Oxidation Catalysis  
Florian Dyckhoff, Technical University Munich, Germany

Cat P-15  Backbone Modified Macrocyclic Tetra-NHC Iron Complexes Applied in Epoxidation Catalysis  
Marco Bernd, Technical University Munich, Germany

Cat P-16  Production of Upgraded Bio-oil from Catalytic Pyrolysis/hydrodexoxygenation and its Emulsification  
Young–Kwon Park, University of Seoul, South Korea

Cat P-17  Water–Soluble, Disulfonated alpha-Diimine Rhodium(I) Complexes: Synthesis, Characterisation and Application as Catalyst Precursors in the Hydroformylation of 1-Octene  
Nikechukwu Nike Omosun, University of Cape Town, South Africa
Comparative study of Chiral Modifiers over Pt Supported on Mesocellular Silica Foam in Enantioselective Hydrogenation
Byeongju Song, Pohang University of Science and Technology, South Korea

The Molecular Characteristics on the Deep HDS and HDN over Alumina and Silica Alumina Supported Metal Catalysts
Joo-Il Park, Hanbat National University, South Korea

Biofuel Additives Production from Glycerol Acetalization over Ni and Co Doped Oxides Catalysts: Experimental Results and DFT Calculations
Alcineia C Oliveira, Universidade Federal do Ceará, Brazil

Corrosion Protection of Mg Based Alloy in Neutral Sodium Chloride Solution by Electrodeposited Ni–TiO₂ – Silane Composite Coating
Mohammad H. Bin Sabt, Kuwait University, Kuwait

Low Cost Advanced Hydrogen Production Platform for On-site Hydrogen Supply
Wang Lai Yoon, Korea Institute of Energy Research, South Korea

P-doped Ni–Fe–S Nanoflowers as a Highly Efficient Electrocatalyst for Oxygen Evolution Reaction
Sangjin Kim, Inha University, South Korea

CoFe₂O₄/β–Ni(OH)₂ Heterojunctioned Composite as an Advanced Electrocatalyst for Oxygen Evolution Reaction
Minsoo Kim, Inha University, South Korea

MOF-Derived Zinc Cobalt Sulfides on N, S Co-Doped Carbon as a Highly Efficient Electrocatalyst for Oxygen Reduction Reaction
Minji Hwang, Inha University, South Korea

In Situ Growth of Nickel-Based Sulfide Nanoneedles on Nickel Foam as a Highly Efficient Bifunctional Electrocatalyst for Oxygen and Hydrogen Evolution Reaction
Dongwook Lim, Inha University, South Korea

Boron ion Doping of Metal-doped Hematite by a Surface Treatment for Enhanced Photoelectrochemical Water Splitting
Hyojin Ahn, German Engineering Research and Development Center LSTME Busan Branch, South Korea

The Effect of Particle Sizes on the Concentration Dependence of the Surface Tension of Aqueous Suspensions of Bentonite
Boris Alchagirov, Kabardino-Balkarian State University named after H.M. Berbekov, Russia

The Influence of Air and its Main Components on the Surface Tension of Mercury
Boris Alchagirov, Kabardino-Balkarian State University named after H.M. Berbekov, Russia

Surface Tension of the Eutectic Alloy PbBi Coolant for Gen–IV In Nitrogen, Oxygen, Atmospheres of Air and in Vacuum
Boris Alchagirov, Kabardino-Balkarian State University named after H.M. Berbekov, Russia

Chemically Modified Biochar Adsorbent for Heavy Metal Removal from the Aqueous Solution
Jin Sun Cha, Korea Testing Laboratory, South Korea
Cat P-32 Removal of Nitrate and Nitrite Contaminants in Wastewater over NiFe$_2$O$_4$ and ZnFe$_2$O$_4$ Nanoparticles
Ndumiso Vukile Mdlovu, Yuan Ze University, Taiwan

Cat P-33 Al Thin film: The Role of Substrate on Film Formation and Morphology
Moojin Kim, Jungwon University, South Korea

Cat P-34 Fabrication of Transition Metal Chalcogenides Alloys for Efficient Water Splitting Electrodes with a Wide pH Range of Electrolyte
Inhwan Oh, Inha University, South Korea

Cat P-35 Effects of Natural Radionuclides on the Processes Occurring in the Environmental Objects: Studying the Cleaning Methods of Water Contaminated with Organic Emissions and the Methods for Cleaning of Soil Contaminated with Heavy Metals and Radionuclides
Khagani Mammadov, Institute of Radiation Problems of Azerbaijan National Academy of Sciences, Azerbaijan

Cat P-36 Improvement of Electrocatalytic Activities and Corrosion Resistance by Carbon Materials for Efficient Hydrogen Evolution Reaction: Graphene, CNT and Carbon Substrates
Ki-Joon Jeon, Inha University, South Korea

Cat P-37 Selective Reduction of CO$_2$ to CO at Room Temperature by Co–N$_4$–Cx Electrocatalyst
Ichiro Yamanaka, Tokyo Institute of Technology, Japan

Cat P-38 Fundamental Analysis of Sulfuric Acid Decomposition on Supported Pt/SiC
Gonzalo Almeida, Chonnam National University, South Korea

Electronic Version

Cat P-39 Electrochemical Detection of H$_2$O$_2$ Based on Iron(cobalt), Nitrogen Co–Doped Porous Carbon
Bin Yan, Nanjing Tech University, China

Cat P-40 Preparation and Hydrogen Evolution Activity of the N–doped Mesoporous Hollow Carbon Spheres Supported Pt Single Atom Electrocatalyst
Panyong Kuang, Wuhan University of Technology, China

Cat P-41 Synthesis of CeO$_2$–ZrO$_2$ Nanosheets and their Enhanced Catalytic Activity in Diesel Soot Oxidation
Zhengzheng Yang, China West Normal University, China

Cat P-42 Magnetic Core–shell Nitrogen–doped Carbon–supported Co$_3$O$_4$ as a Highly–reactive Nanoreactor for the Catalytic Degradation of Bisphenol A
Liu Fuqiang, Nanjing University, China

Cat P-43 Environment–friendly Catalyst for Simultaneous Removal of Nitrogen Oxides and Mercury
Qijie Jin, Nanjing Tech University, China

Cat P-44 Fundamental Analysis of Sulfuric Acid Decomposition on Supported Pt/SiC
Gonzalo A. Almeida, Chonnam National University, Korea

Cat P-45 MnO$_2$–encapsulated CeO$_2$ Nanorod Supported iron–based Catalyst for High–temperature Fischer–Tropsch Synthesis of Light Olefins
Xian Wu, University of Science and Technology, China
Session I | Energy  
Catalysis and Energy | Catalysis for Renewable Sources | Catalysis in Oil and Gas  

**Chairs:**  
Juha Lehtonen, VTT Technical Research Centre of Finland, Finland  
Avinashkumar V Karre, Worley, Baton Rouge, LA

**08:00-08:20**  
Synthesis and Characterization of PDVB–based Solid Acid Catalysts for Biodiesel Production via Transesterification of Palmitic Oil  
You-Sheng Lin, Yuan Ze University, Taiwan

**08:20-08:40**  
CO$_2$/CO Hydrogenation for the Production of Lighter Hydrocarbons over Bifunctional Co/SAPO–34 Catalyst  
Hyun Dong Kim, Clean Energy Research Center, KIST, South Korea

**08:40-09:00**  
First Principles Evaluation on Catalysis of Oxygen Evolution and Fuel Production in an Artificial Photosynthesis System  
Che-Wun Hong, National Tsing Hua University, Taiwan

**09:00-09:20**  
Laser Ablation Synthesis in Solution–Galvanic Replacement Reaction (LASiSGRR): A Facile Route for Synthesizing Intermetallic Nanoalloys and Hybrid Nanocomposites as Efficient Electrocatalysts  
Dibyendu Mukherjee, University of Tennessee, Knoxville, TN

**09:20-09:40**  
In Situ Grown Metal Nanoparticle Catalysts: Properties and Control  
Tae-Sik Oh, Auburn University, Auburn, AL

**09:40-10:00**  
First-Principles Study of Catalytic CO$_2$/Water Decomposition on Layered Materials  
Hong Seok Kang, Jeonju University, South Korea

**10:00-10:20**  
Catalysis for Biomass Conversion to Transportation Fuel Compounds  
Juha Lehtonen, VTT Technical Research Centre of Finland, Finland

**10:20-10:40**  
Pulsed–Laser in Liquids Preparation of Clean–Energy Nanomaterials  
Astrid M. Mueller, University of Rochester, Rochester, NY

**10:40-11:00**  
Networking Break  
@ San Diego BallRoom

**11:00-11:20**  
Catalytic Oxidation of Benzothiophenes Using a Pyridinium Ionic Liquid  
Yan Zhang, Memorial University of Newfoundland, Canada

**11:20-11:40**  
Han-Wei Chang, National United University, Taiwan

**11:40-12:00**  
Modifying Fischer–Tropsch Reaction Sequence with Addition of Zeolite to Iron–based Activated–Carbon Supported Catalyst  
Avinashkumar V Karre, Worley, Baton Rouge, LA

**12:00-12:20**  
Chemicals Production by Methylation of Monoaromatic Lignin Depolymerization Products  
Isabel Vicente Valverde, Eurecat Technological Center of Catalonia, Spain
12:20–12:40  Dimethyl Ether Production by Catalytic Dehydration of Methanol Using Metal–Transition Chalcogenides Supported on Silica–Aluminates Nanomaterials
Marco Antonio Alvarez Amparan, Centro de Investigación Científica y de Educación Superior de Ensenada (CICESE), Baja California, México / CNyN–UNAM

12:40–13:00  In situ X–Ray Spectroscopic Studies of Energy Sciences
Chung–Li Dong, Tamkang University, Taiwan

13:00–14:00 Networking Lunch @ San Diego BallRoom

Young Researchers Forum

14:00–14:15  Highly Dispersed Cobalt Nano Particles Encapsulated in Hollow Silicalite–1 for Fischer–Tropsch Synthesis
Xin Li, North Carolina A&T State, University, Greensboro, NC

14:15–14:30  Fischer–Tropsch Studies with CoRu–based Catalysts Supported by Mesoporous Composite Oxide Support in a 3D–Printed Stainless Steel (SS) Microreactor
Sujoy Bepari, North Carolina A&T State, University, Greensboro, NC

14:30–14:45  Experimental Study of Supported Catalysts for the Steam Reforming of Acetic Acid
Marta Cortese, University of Salerno, Italy

14:45–15:00  Selective Production of Greener Fuel from Castor Oil Using a Fe–Pd–Ni Trimetallic Single Atom Alloy Catalyst Encapsulated in Disordered Worm like SiO$_2$–TiO$_2$ Hybrid Support via Hydrodeoxygenation in Hexane Containing Pressurized CO$_2$
Saurav Bhattacharjee, National Tsing Hua University, Taiwan

15:00–15:15  Improved Catalytic Performance of Modified Nickel–Based Catalysts in Combined Steam and Dry Reforming of Methane (CSDRM)
Nichakorn Buasuk, Chulalongkorn University, Thailand

Zhenyu Zhang, Colorado School of Mines, Golden, CO

15:30–15:45  Effect of Sr on Catalytic Properties of MgAlO Catalyst in Ethanol Dehydrogenation
Patchaporn Seekhiaw, Chulalongkorn University, Thailand

15:45–16:00 Networking Break @ San Diego BallRoom

16:00–16:15  An Initial study of Biogas Upgrading to Bio–Methane with Carbon Capture Using Nano–structured Ceramic Membranes
Priscilla Ogunlude, Robert Gordon University, UK

16:15–16:30  Quantitative Mapping of Carbon and Metals on Catalysts Down to the PPM Scale by Laser Induced Breakdown Spectroscopy (LIBS)
Lina Jolivet, IFP Energies Nouvelles, France

16:30–16:45  Synthesis and Characterization of CuO Nanostructures as an Electrode Material for Supercapacitors
Neha Paras, National Institute of Technology, Kurukshetra, India
Session II | MATERIALS

Material Sciences | Nanocatalysis | Polymer Engineering

@ Los Angeles Room

Chairs: Peter J. Schubert, Indiana University–Purdue University Indianapolis, Indianapolis, IN
        Xiujun (James) Li, University of Texas at El Paso, El Paso, TX
        Herman S. Mansur, Universidade Federal de Minas Gerais, Brazil

08:00–08:20  Heterogeneous Nucleation of Aluminum on Al₃Ti Phases with Tetragonal D₀₂₂ Structure and L₁₂ Modified Structure
Yoshimi Watanabe, Nagoya Institute of Technology, Japan

08:20–08:40  Integration of Nanoscale Gold into Polymer Particles for a Highly Selective and Reactive Quasi-Homogeneous Catalyst
Hongsik Byun, Keimyung University, South Korea

08:40–09:00  Design of Bimetal Catalyst for VOC Removal from Industrial Waste Air
Natasa Novak Tusar, National Institute of Chemistry, Slovenia

09:00–09:20  Fundamental Electrochemical Insights of Vertically Aligned Carbon Nanofiber Architecture as a Novel Catalyst Support for ORR
Jun Li, Kansas State University, Manhattan, KS

09:20–09:40  Facile Synthesis of NHC-Stabilized Metal Nanoparticles and their Catalytic Application in Selective Hydrogenations
Miriam Diaz de los Bernardos Sánchez, Eurecat Technological Center of Catalonia, Spain

09:40–10:00  Novel Hybrid Nanozyme–Catalysts for Ferroptosis–Induced Cancer Therapy Based on Polysaccharide–Enzyme–Magnetic Iron Oxide Nanostructures
Herman S. Mansur, Universidade Federal de Minas Gerais, Brazil

10:00–10:20  Syngas Production from Hydrocarbons on Ni–Based Catalysts: Strategy to Enhance Thermal Stability of Ni Nanoparticles
Jong Wook Bae, Sungkyunkwan University, South Korea

10:20–10:40  Visible–Light Water Oxidation by Polyoxometalate Complexed Metal–Oxide Cores
Ira Alan Weinstock, Ben–Gurion University of the Negev, Israel

10:40–11:00  Networking Break

11:00–11:20  Catalytically Modulated Memristor
Peter J. Schubert, Indiana University–Purdue University Indianapolis, Indianapolis, IN

11:20–11:40  Mechanism of Metal–Metal Cooperation in Sonogashira Coupling: Learning from Highly Dynamic PdII–CuI Tetrametallic Assemblies
Agustí Lledos, Universitat Autònoma de Barcelona, Spain

11:40–12:00  Molecularly Imprinted Nanoparticles as Artificial Enzymes for Efficient and Selective Catalysis in Water
Yan Zhao, Iowa State University, Ames, IA

12:00–12:20  The Generation of H₂ vs Hydrogenation of Substrates: On the Way to Green Chemistry
Albert Poater, Universitat de Girona, Spain

Olumide Ayodele, International Iberian Nanotechnology Laboratory, Portugal

12:40–13:00  Catalytic Surfaces Under Reaction Conditions Observed by in–situ Synchrotron Technique
Yan–Gu Lin, National Synchrotron Radiation Research Center, Taiwan

13:00–14:00  Networking Lunch

@ San Diego BallRoom
14:00–14:20 Catalysis with Liquid Metal Alloys
Christian Papp, University of Erlangen–Nuremberg, Germany

14:20–14:40 Precursor Influence on Flame Made Hopcalite Nanoparticles for Low–Temperature CO Oxidation Under Humid Conditions
Grothe Julia, Technische Universität Dresden, Germany

14:40–15:00 Downsizing Nanoparticles to Supported Single Metal Atoms Catalysts: in situ Studies to Understand and Stabilize a Rational Design to Improve Catalytic Systems
Debora M. Meira, CLS@APS, Advanced Photon Source, Argonne National Laboratory, IL

15:00–15:20 Strong Interaction Between Au Nanoparticles and Porous Polyurethane Sponge Enables Efficient Environmental Catalysis with High Reusability
Xiujun (James) Li, University of Texas at El Paso, El Paso, TX

15:20–15:40 Liquid Phase Catalytic Oxidation of Cyclohexane Using Advanced Oxidation Process
VSR Rajasekhar Pullabhotla, University of Zululand, South Africa

15:40–16:00 Development of Conductive Cotton for Energy Harvesting and Photocatalytic Applications
Sompit Wanwong, King Mongkut’s University of Technology Thonburi, Thailand

16:00–16:20 DFT Study on the Mechanism of H₂ Oxidation by Bio–inspired Binuclear Catalyst
Miho Isegawa, Kyushu University, Japan

16:20–16:40 Synthesis of Multi–metallic Subnanocatalysts by Using Dendrimer Reactors
Kimihisa Yamamoto, Tokyo Institute of Technology, Japan

16:40–17:00 Networking Break @ San Diego BallRoom

Young Researchers Forum

17:00–17:15 Advanced Characterization of Transition Metals on TiO₂ Nanoparticles Under Catalytic Reaction: The Role of Interface and Subsurface Oxygen in CO₂ and CO Conversion
Djawhar Ferrah, University of California, Irvine, CA

17:15–17:30 Gold Nanoparticles Supported on Metal Oxide Based Nanotubes for the Catalytic Reduction of Nitroarenes
Shanmugaraj Krishnamoorthy, Universidad de Concepción, Chile

17:30–17:45 Kerosene Removal from Water Using TiO₂, V₂O₅ and MnO₂ Nanoparticles Modified MWCNTs
Thamer A. Abdullah, University of Pannonia, Hungary

17:45–18:00 Hydrogenation of Polyethylene Terephthalate to Environmentally Friendly Products over a Vulcan XC–72 Carbon Supported Mono and Bimetallic Heterogeneous Catalysts in Greener Reaction Systems
Avinash B. Lende, National Tsing Hua University, Taiwan

18:00–18:15 Effect of Co–Catalyst Combination on Ti-Based Ziegler–Natta Catalyst in Gas–Phase Ethylene Polymerization
Thanyporn Pongchan, Chulalongkorn University, Thailand

18:15–18:30 Preparation of WO₃–Based Catalysts on Silica and Silica–alumina Supports for Propene Self–Metathesis
Nattaphon Hongrutai, Chulalongkorn University, Thailand
### Session III | INDUSTRY

**Reaction Engineering | Simulation & Modeling | Surface & Colloids | Fluid Dynamics | Quantum Chemistry | Environmental Catalysis**

**Chairs:**
- Olalla Nieto Faza, Universidade de Vigo, Spain
- Helene GERARD, Sorbonne University, Paris, France

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<tr>
<th>Time</th>
<th>Session</th>
<th>Title</th>
<th>Speaker</th>
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<tbody>
<tr>
<td>08:00-08:20</td>
<td></td>
<td>Synthetic Chemistry: The Quest for Predictive Simulations</td>
<td>Martin Jaraiz</td>
<td>University of Valladolid, Spain</td>
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<td>08:20-08:40</td>
<td></td>
<td>Understand the Mutational Effect and Substrate Promiscuity in Enzyme Catalysis: Pre-Reaction State and QM/MM Calculation</td>
<td>Yilei Zhao</td>
<td>University of California, Los Angeles, CA</td>
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<td>08:40-09:00</td>
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<td>Preparation of Carbonaceous Ion-exchangers for Water Purification</td>
<td>Motoi Machida</td>
<td>Chiba University, Japan</td>
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<td>09:00-09:20</td>
<td></td>
<td>Enzyme as Powerful Biocatalyst for Precision Synthesis of Functional Polysaccharide Materials</td>
<td>Jun-ichi Kadokawa</td>
<td>Kagoshima University, Japan</td>
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<td>09:20-09:40</td>
<td></td>
<td>Methane to Ethane Conversion by Liquid Metal Indium: A DFT Mechanistic Study</td>
<td>Jun-ya Hasegawa</td>
<td>Hokkaido University, Japan</td>
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<td>09:40-10:00</td>
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<td>Magnesium Oxide Enhancement of the Catalytic Performance of Nickel Supported on Gamma-Alumina Doped with Silica in Dry Reforming of Methane</td>
<td>Abdulaziz Bagabas</td>
<td>King Abdulaziz City for Science and Technology, Saudi Arabia</td>
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<td>10:00-10:20</td>
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<td>Dry Reforming of Methane to Syngas over Nanostructured La2O3-Al2O3-Supported PtMo Nanoparticles</td>
<td>Alcineia C Oliveira</td>
<td>Universidade Federal do Ceará, Brazil</td>
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<td>10:20-10:40</td>
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<td>Copper Catalyzed C-C Bond Formation: Intertwined Theoretical and Experimental Approaches</td>
<td>Helene GERARD</td>
<td>Sorbonne University, Paris, France</td>
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<td>10:40-11:00</td>
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<td>Networking Break</td>
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<td>@ San Diego BallRoom</td>
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<td>11:00-11:20</td>
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<td>Selective Mono-Alkylbenzene Disproportionation over Silylated MFI Zeolite</td>
<td>Tseng-Chang Tsai</td>
<td>National University of Kaohsiung, Taiwan</td>
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<td>11:20-11:40</td>
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<td>Quantum Effects on the Diffusivity of Hydrogen Isotopes in Zeolites</td>
<td>Marcos Salazar</td>
<td>Université de Bourgogne, France</td>
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<td>11:40-12:00</td>
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<td>Heterogeneous Photocatalysis and Photo-Fenton Technologies as Alternatives for UV-Filters Removal</td>
<td>Henry Zuniga-Benitez</td>
<td>Universidad de Antioquia UdeA, Colombia</td>
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<td>12:00-12:20</td>
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<td>Computational Mechanistic Insights into Deoxygenation Reactions for Biomass Valorization</td>
<td>Olalla Nieto Faza</td>
<td>Universidade de Vigo, Spain</td>
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<td>12:20-12:40</td>
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<td>Using Atom-in-Material Descriptors to Better Understand Catalysts</td>
<td>Thomas A. Manz</td>
<td>New Mexico State University, Las Cruces, NM</td>
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<td>12:40-13:00</td>
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<td>HCl Emission Minimization via. Unit Operations and Chemical Reaction Modification</td>
<td>Rahul Patil</td>
<td>Speciality Chemicals (MNC), Sugar Land, TX</td>
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<td>13:00-14:00</td>
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<td>Networking Lunch</td>
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<td>@ San Diego BallRoom</td>
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<td>14:00-14:20</td>
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<td>Phenol Removal in Seawater by Heterogeneous Photocatalysis Using TiO2- Modified Activated Carbon Materials</td>
<td>Yvan Jesus Olortiga Asencios</td>
<td>Universidade Federal de São Paulo, Brazil</td>
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Performance of Acacia Gum as a Novel Additive in Thin film Composite Polyamide RO Membranes
Yehia Manawi, QEERI, Qatar

Unraveling a Homogeneous Route to Glycerol Valorization
Marco Nascimento, Cidade Universitária, Brazil

Catalytic pyrolysis of methane: An experimental and Technoeconomic analysis for Hydrogen and Carbon Co-Production
Jarrett Riley, U.S. Department of Energy, Morgantown, WV

15:20–15:35  Oxidation of Propene on Pt/$\gamma$-Al$_2$O$_3$ Prepared by Supercritical Deposition for Aftertreatment Systems of Heavy-Duty Diesel Engines
Selmi Erim Bozbag, Koç University, Turkey

15:35–15:50  High Conductive Structured Catalysts for CO2 Methanation Process Intensification
Simona Renda, University of Salerno, Italy

15:50–16:05  Effect of Solvation on the Reactivity of Co$_3$O$_4$ (001) (001) Surface: Insights from Molecular Dynamics Simulations
Stephane Kenmoe, Universitaet Duisburg-Essen, Germany

16:05–16:20  Networking Break  @ San Diego BallRoom

Karen Villegas Dominguez, Université de Sherbrooke, Canada

16:35–16:50  Study on the Reaction Mechanisms for DME Synthesis from Syngas Using Computational Chemistry and Microkinetic Model
Jongmin Park, Seoul National University, South Korea

16:50–17:05  Synergistic Bimetallic Pd–Pt/TiO$_2$ Catalysts for Hydrogenolysis of Xylitol with In-Situ Formed H$_2$: Structure–Sensitivity Study and Kinetic Analysis
Jian Shen, China Pacific Northwest National Laboratory, USA
Session IV: TYPES of CATALYSIS  @ California BallRoom A&D

Photocatalysis | Electrocatalysis

Chairs: Mal-Soon Lee, Pacific Northwest National Laboratory, Richland, WA
       Meng Li, Idaho National Laboratory, Idaho Falls, ID

08:00-08:20 Photoredox Catalysts for Direct Phenol Production from Benzene
            Kei Ohkubo, Osaka University, Japan

08:20-08:40 Hydrogen Evolution by Photocatalytic Splitting of Water Using SrTiO₃/PAN Based Fibers
            Gulmira Yar-Mukhamedova, Al-Farabi Kazakh National University, Kazakhstan

08:40-09:00 Synthesis and Photocatalytic Performance of Core/Shell Structure Rutile@Anatase TiO₂ Nanofibers
            Ming-Chung Wu, Chang Gung University, Taiwan

09:00-09:20 Photoassisted Degradation of Rhodamine B and Caffeine by Synthesis of ZnO/Hydroxyapatite Nanoparticles
            Abdelhak Kherbeche, Université Sidi Mohammed Ben Abdellah, Morocco

09:20-09:40 Photocatalysis of Plasmon Resonant Nanostructures and Two-Dimensional Materials
            Stephen B. Cronin, University of Southern California, Los Angeles, CA

09:40-10:00 Valorisation of Biomass by Hydrothermal Transformation and Photocatalysis
            Guillard Chantal, University Lyon 1, France

10:00-10:20 Revisiting the Universal Behavior of Oxides for Oxidative Catalysis
            Michal Bajdich, SUNCAT Center for Interface Science and Catalysis, Menlo Park, CA

10:20-10:40 Enhanced Electrochemical Hydrogenation of Biomass Derived Organic Compounds
            Mal-Soon Lee, Pacific Northwest National Laboratory, Richland, WA

10:40-11:00 Networking Break  @ San Diego BallRoom

11:00-11:20 From Hydrogen Production to its Utilization: Developing Electrocatalysts for Water Splitting and Hydrogenation Reactions
            Bin Hua, Idaho National Laboratory, Idaho Falls, ID

11:20-11:40 Constructing Heterostructured Nanocatalysts for Solid State CO₂ Electrolyzer
            Meng Li, Idaho National Laboratory, Idaho Falls, ID

11:40-12:00 Innovative Antibacterial Surfaces Based on Photocatalytic Nanostructures for Water Quality Technology
            Begoña Espiña, INL – International Iberian Nanotechnology Laboratory, Portugal

12:00-12:20 Plasmonically Enhanced Electrocatalyst Design for CO₂ Reduction
            Jeff Urban, Berkeley Lab, Emeryville, CA
12:20–12:40 Engineering Precious Metal-free Catalyst Interfaces by Electrografting for Energy Applications
Loic Assaud, University of Paris–Sud, France

12:40–13:00 Preparation of Multifunctional Carbon-Based Supported Nano Titania Photocatalyst for Water Clarification
Ilker Erdem, Abdullah Gül University, Turkey

13:00–13:20 Copper-Based Electrocatalyst Derived from a Copper Chelate Polymer for Oxygen Reduction Reaction in Alkaline Solutions
Izabela I. Rzeznicka, Shibaura Institute of Technology, Japan

13:20–14:20 Networking Lunch @ San Diego BallRoom
Young Researchers Forum

14:20–14:35 1D TiO$_2$ Nanotube Layers Decorated by Atomic Layer Deposition: Efficient Photocatalyst
Martin Motola, University of Pardubice, Czech Republic

14:35–14:50 Photocatalytic Behaviour of B–Site Modified Photoferroic Fe–Doped Barium Titanate Nanoparticles
Ifeanyichukwu Amaechi, Institut National de la Recherche Scientifique, Canada

14:50–15:05 Hot Electron Driven Photocatalysis on Plasmon–resonant Grating Nanostructures
Yu Wang, University of Southern California, Los Angeles, CA

15:05–15:20 Cellulose Nanofiber/Titanium dioxide Nanowire Film for Reusable Organic Pollutant Photodegradation
Yin-Hsuan Chang, Chang Gung University, Taiwan

15:20–15:35 Construction of 2D/1D g- C$_3$N$_4$/TiO$_2$ with Z-Scheme Heterostructure for Efficient Water Splitting
Ting-Han Lin, Chang Gung University, Taiwan

15:35–15:50 Formulation and Characterization of W-Doped Titania Nanotube for Adsorption/Photodegradation of Methylenes Blue and Basic Violet 3 Dyes
Vukile Mdlovu, Yuan Ze University, Taiwan
### Session V | CHEMICAL SYNTHESIS

Chemical Kinetics | Biocatalysts | Nanochemistry | Organometallics Chemistry

**Chairs:**
- **Tuulamari Helaja**, VTT Technical Research Centre of Finland, Finland
- **Anderson Bonon**, HORIBA Scientific, Piscataway, NJ

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<th>Time</th>
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| 08:00-08:20 | Applications of Iridium Complexes with Heterodonor Carbene-Based Ligands in Catalysis. From Water Oxidation to Asymmetric Hydrogenation
  **Oscar Pamies**, Universitat Rovira i Virgili, Spain |
| 08:20-08:40 | Improved Generations of Catalysts for the Preparation of Challenging High Value Chiral Compounds
  **Montserrat Dieguez**, Universitat Rovira i Virgili, Spain |
| 08:40-09:00 | Boronated Organometallic Complexes for Non-Aqueous Flow Batteries
  **Emmanuelle Despagnet-Ayoub**, Occidental College, Los Angeles, CA |
| 09:00-09:20 | Gold, Silver, and Serendipity in Catalyst Development
  **Anna G. Wenzel**, Pitzer College, Claremont, CA |
| 09:20-09:40 | VTT Sugar Acid Pathway to FDCA
  **Tuulamari Helaja**, VTT Technical Research Centre of Finland, Finland |
| 09:40-10:00 | A Generalized Kinetic Framework Applied to Whole-Cell Bioelectrocatalysis in Bioflow Reactors Clarifies Performance Enhancements for Geobacter Sulphurreducens Biofilms
  **Jesse Greener**, Laval University, Canada |
| 10:00-10:20 | Oxo-Molybdenum Catalysed Conversion of Vicinal Diols to Olefins
  **Alex John**, California State Polytechnic University, Pomona, CA |
| 10:20-10:40 | Synthesis and Purification of Limonene Diepoxide via Green Catalytic Epoxidation: Conversion, Selectivity Optimization and Characterization
  **Anderson Bonon**, HORIBA Scientific, Piscataway, NJ |
| 10:40-10:50 | Networking Break @ San Diego BallRoom |
| 10:50-11:10 | Palladium-Catalyzed Hydroformylation Using Formaldehyde as Syngas Surrogate: Mechanistic and Kinetic Insights
  **Aitor Gual Gozalbo**, Eurecat Technological Center of Catalonia, Spain |
| 11:10-11:30 | Production of Glycerol Carbonate from Glycerol over Modified Sodium Aluminate Catalysts
  **Anusorn Seubsai**, Kasetsart University, Thailand |
| 11:30-11:50 | Glycerol Carboxylation Using Zinc-Based Metal Organic Framework with Lanthanum Incorporation
  **Chechia Hu**, Chung Yuan Christian University, Taiwan |
| 11:50-12:10 | Effect of Oxygen Concentration in the Fuel Combustion Mix Inside Furnaces
  **Freddy X. Jervis**, Escuela Superior Politecnica del Litoral, Ecuador |

**Young Researchers Forum**

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  **Jonas Schlagintweit**, Technical University Munich, Germany |
| 12:25-12:40 | Preparation of Supported Catalysts for the Production of 2,3-dimethylbutenes Using Olefin Metathesis, Selective Hydrogenation and Dehydrogenation Reactions
  **Isaias Barbosa Aragao**, Université Lyon 1, France |
12:40–12:55  Catalytic Cracking of Date Palm Lignocellulosic Waste to High Value Chemicals using Commercial NiAl Alloy Catalyst
Emmanuel Galiwango, United Arab Emirates University, UAE

12:55–13:10  TiO2/Ni Nanostructure Protected GaAs for Photoelectrochemical Hydrogen Production
Mahdi Alqahtani, King Abdulaziz City for Science and Technology (KACS), Saudi Arabia

13:10– Lunch & Departures  @ San Diego BallRoom

Notes: ______________________________________________________________________
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We wish to see you at
CCE-2021
San Francisco

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Email: catalysis@uniscigroup.org
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