5th International Conference on

# Catalysis and Chemical Engineering

CCE-2021

February 22-26, 2021 | Virtual

Last updated: January 26, 2021

**Presentation Slots are Available. Book your Slot at:**
https://catalysis.unitedscientificgroup.org/registration_form

## Day 1 | February 22, 2021

| | |
|---|---|
| 08:00-08:05 | Introduction: Prof. Mannar Ram Maurya, Indian Institute of Technology Roorkee, India |

## Keynote Presentation

| Meeting Timezone (EST) | Local Time | |
|---|---|---|
| 08:05-08:35 | 18:35-19:05 | Dioxidomolybdenum(VI) Complexes Supported on Chloromethylated Polystyrene as Catalyst for Oxidative Transformations |
| | | **Mannar Ram Maurya,** Indian Institute of Technology Roorkee, India<br>**H-Index:** 45 |

Dr. James J. Spivey is the J. M. Shivers and C.M. Eidt,Jr. Professor of Chemical Engineering at Louisiana State University. He is Editor-in-Chief of Catalysis Today, and Editor of the Royal Society of Chemistry's Catalysis book series. He has written/edited a total of 17 books over the last 15 years, and has authored more than 100 publications. He has managed over $30 million in sponsored projects over the past 20 years. He is past Director of the Center for Atomic-level Catalyst Design at LSU one of 46 multi-million-dollar DOE Energy Frontier Research Centers.

## Plenary Lectures

| Meeting Timezone (EST) | | |
|---|---|---|
| 08:35-09:10 | | **James J. Spivey,** Louisiana State University, Baton Rouge, LA, USA<br>**H-Index:** 56, **Editor In-Chief:** Catalysis Today |

Dr. James J. Spivey is the J. M. Shivers and C.M. Eidt,Jr. Professor of Chemical Engineering at Louisiana State University. He is Editor-in-Chief of Catalysis Today, and Editor of the Royal Society of Chemistry's Catalysis book series. He has written/edited a total of 17 books over the last 15 years, and has authored more than 100 publications. He has managed over $30 million in sponsored projects over the past 20 years. He is past Director of the Center for Atomic-level Catalyst Design at LSU one of 46 multi-million-dollar DOE Energy Frontier Research Centers.

| Meeting Timezone (EST) | Local Time | |
|---|---|---|
| 09:10-09:45 | 08:10-08:45 | **Tobin J. Marks,** Northwestern University, Evanston, IL, USA<br>**H-Index:** 180, **Wikipedia:** https://en.wikipedia.org/wiki/Tobin_J._Marks |

Professor Tobin J. Marks is currently Charles E. and Emma H. Morrison Professor of Chemistry, Professor of Materials Science and Engineering and Vladimir N. Ipatieff Professor of Catalytic Chemistry at Northwestern University, Evanston, IL. Recent publications cover topics of f-element hydroelementation, supported catalysts, and bimetallic catalysis. Prof. Marks has received uncountable number of awards, and he is the member of National Academy of Engineering and Science. His awards includes: ACS Priestley Medal, Harvey Prize in Science & Technology from the Technion in Israel, Sacconi Medal, Italian Chemical Society, Materials for Industry Award, Royal Society of Chemistry UK, Honorary Foreign Member, Chinese Chemical Society, Einstein Award, Chinese Academy of Sciences, Member, National Academy of Inventors, Gabor A. Somorjai Award for Creative Research in Catalysis and many more.

| Meeting Timezone (EST) | Local Time | |
|---|---|---|
| 09:45-10:20 | 09:45-10:20 | **Craig L. Hill,** Emory University, Atlanta, GA, USA<br>**H-Index:** 92, **Wikipedia:** https://en.wikipedia.org/wiki/Craig_L._Hill |

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 nanoscale materials and POM derivatives. 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).

**10:20-10:30** **Break**

## Keynote Presentations

| Meeting Timezone (EST) | Local Time | |
|---|---|---|
| 10:30-11:00 | 10:30-11:00 | Molecular Catalysis Covering H2, O2, and H2O Activation with Porphyrins, Chlorins, and Corroles<br><br>**Dilek Dogutan**, Harvard University, Cambridge, MA, USA |

Dilek Dogutan Kiper is the Principal Research Scientist for the Nocera Lab at Harvard, which focuses on renewableenergy research and solutions. Under her leadership, the Group has participated in numerous Green Lab competitions and pilots, demonstrating how energy-intensive labs can maximize energy reduction opportunities while strengthening their cutting-edge research.

| Meeting Timezone (EST) | Local Time | |
|---|---|---|
| 11:00-11:30 | 10:00-10:30 | **Kenneth M. Nicholas,** University of Oklahoma, Norman, OK, USA |

Kenneth M. Nicholas, George Lynn Cross Research Professor Emeritus in the Department of Chemistry and Biochemistry at the University of Oklahoma, is the winner of the 2019 Oklahoma Chemist Award for his outstanding contributions to the discovery, fundamental understanding, and applications of chemical reactions promoted by transition metal compounds.

| Meeting Timezone (EST) | Local Time | The Roles of HCO3-/CO-32- In Catalytic Oxidation Processes |
|---|---|---|
| 11:30-12:00 | 18:30-19:00 | **Dan Meyerstein,** Ariel University & Ben-Gurion University, Israel<br>**H-Index:** 45, **Wikipedia:** https://en.wikipedia.org/wiki/Dan_Meyerstein |

Prof. (Emeritus) Dan Meyerstein, of BGU's Department of Chemistry and currently President of the Ariel University Center of Samaria, recently became a member of the Academia Europaea. He is the member of Israel Chemical Society, Israel Society for Oxygen and Free Radical Research. American Chemical Society, the Royal Society of Chemistry and the Society for Biological Inorganic Chemistry. He has received1998 Kolthoff prize and 1997 Meitner-Humboldt Research Prize.

| Meeting Timezone (EST) | Local Time | From Homogenous to Heterogenous Energy-Relevant Electrocatalysis by Substituent-Free N4 Macrocyclic Metal Complexes |
|---|---|---|
| 12:00-12:30 | 19:00-19:30 | **Gross Zeev,** Technion, Israel<br>**H-Index:** 65, **Wikipedia:** https://en.wikipedia.org/wiki/Dan_Meyerstein |

Zeev Gross received his PhD in chemistry from Bar-Ilan University in 1988, in the field of physical organic chemistry. He then moved to Princeton University for two years as a Fulbright postdoctoral fellow, during which he explored several aspects of metalloporphyrin chemistry with Professor J. T. Groves as mentor. He was a Moore Distinguished Scholar at Caltech in 2013, received the Israel Chemical Society Award for the Outstanding Scientist in 2014, and was selected to get the Hans Fischer carrier award in 2018.

| Meeting Timezone (EST) | Local Time | Structured (Micro)Reactors for Catalysis |
|---|---|---|
| 12:30-13:00 | 18:30-19:00 | **Jacob A. Moulijn,** Delft University of Technology, The Netherlands<br>**H-Index:** 127 |

Jacob A. Moulijn is Emeritus Professor of Chemical Engineering at the Delft University of Technology (1990-2007). At present he serves as part-time Professor at the same university and as an Honorary Visiting Professor at Cardiff University. In addition to that he is active as a consultant, in particular in the field of biomass conversion. He specialised in Catalysis Engineering. He was Full Professor at the University of Amsterdam (1986-1990), visiting professor at several universities and active in China for the UN.

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|---|---|
| **13:00-13:30** | **Break** |

| Meeting Timezone (EST) | Local Time | Graphene Based Metal Oxide Controlled Nanocomposites for Enhanced Photocatalytic Activity |
|---|---|---|
| 13:30-14:00 | 15:30-14:00 | **Martin Schmal,** Federal University of Rio De Janeiro, Brazil<br>**H-Index:** 50 |

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.

| Meeting Timezone (EST) | Local Time | **Debbie C. Crans,** Colorado State University, Fort Collins, CO, USA |
|---|---|---|
| 14:00-14:30 | 12:00-12:30 | **Wikipedia:** https://en.wikipedia.org/wiki/Debbie_C._Crans |

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.

| Meeting Timezone (EST) | Local Time | **Francisco Zaera,** University of California, Riverside, CA, USA |
|---|---|---|
| 14:30-15:00 | 11:30-12:00 | **H-Index:** 81 **Wikipedia:** https://en.wikipedia.org/wiki/Francisco_Zaera |

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.

| Meeting Timezone (EST) | Local Time | **Angela K. Wilson,** Michigan State University, East Lansing, MI, USA |
|---|---|---|
| 15:00-15:30 | 15:00-15:30 | **H-Index:** 44 **Wikipedia:** https://en.wikipedia.org/wiki/Angela_K._Wilson |

Angela K. Wilson is an American computational, theoretical, and physical chemist. She is currently the John A. Hannah Distinguished Professor of Chemistry in the department of chemistry of Michigan State University. Previously she was professor of computational chemistry and co-director of the Center for Advanced Scientific Computing and Modeling (CASCaM) at the University of North Texas. She was Associate Vice Provost for Faculty at the University of North Texas, where she led the Office of Faculty Success, working with ~2,400 faculty through February 2016, when she moved to Michigan State University (MSU). In March 2016, Wilson began a position as the Chemistry Division Director of the National Science Foundation, while concurrently on the MSU faculty.

# Plenary Lectures

| Meeting Timezone (EST) | Local Time | |
|---|---|---|
| 15:30-16:05 | 12:30-13:05 | **Gabor A. Somorjai,** University of California at Berkeley, Berkeley, CA, USA<br>**Wikipedia:** https://en.wikipedia.org/wiki/G%C3%A1bor_A._Somorjai |

Professor 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 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. 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.

**16:05-16:15** **Break**

| Meeting Timezone (EST) | Local Time | |
|---|---|---|
| 16:15-16:50 | 13:15-13:50 | **William Andrew Goddard III,** California Institute of Technology, Pasadena, CA, USA<br>**H-Index:**166 **Wikipedia:** https://en.wikipedia.org/wiki/William_Andrew_Goddard_III |

Professor 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 Presentations

| Meeting Timezone (EST) | Local Time | |
|---|---|---|
| 16:50-17:20 | 16:50-17:20 | **Debasish Kuila,** North Carolina A&T State University, Greensboro, NC, USA<br>**H-Index:**20 |

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.

| Meeting Timezone (EST) 17:20-17:50 | Local Time 06:20-06:50 February 23, 2021 | Recent Developments and Challenges in Practical Application of Visible–Light–Driven TiO2–Based Heterojunctions for Photocatalytic Degradation of Emerging Pollutants |
|---|---|---|
| | | **Irene Man Chi Lo,** HKUST, Hong Kong |

Prof. Irene LO received her PhD degree in Civil (Environmental) Engineering from the University of Texas at Austin in 1992. She was also Adjunct Professor of Tongji University, Tianjin University, Jilin University and Harbin Institute of Technology in China. She had been Visiting Professor of Technical University of Denmark and the University of Wisconsin at Madison. Prof. Lo has been appointed as a Justice of Peace (JP) by the Government of the Hong Kong Special Administrative Region in 2017.

## Special Talk

| Meeting Timezone (EST) 17:50-18:50 | Local Time 17:50-18:50 | Catalysis and Novel Synthesis of Nanostructured Materials |
|---|---|---|
| | | **William R. Moser,** Worcester Polytechnic Institute, Worcester MA, USA |

Dr. Moser is currently Professor Emeritus in the Chemical Engineering Department of the Worcester Polytechnic Institute. After being awarded a Ph.D. in Chemistry at MIT he was a staff scientist in homogeneous catalysis at the Organometallic Institute in Zurich. After returning to the US, he worked at the Exxon Corporate Labs and Badger-Raytheon Corporate Labs before joining the Chemical Engineering faculty at WPI.
He was a member of the WPI Center for Inorganic Membrane Catalysis and served as President of the Organic Reactions Catalysis Society, New York Academy of Sciences Catalytic Division, The New England Catalysis Society, Catalytic Technology Inc., and director of the ACS Petroleum Division.

# Day 2 | February 23, 2021

## Session I: Energy

**Catalysis and Energy | Catalysis for Renewable Sources | Catalysis in Oil and Gas**

| Meeting Timezone (EST) | Local Time | Chairs: To be Announced |
|---|---|---|
| 07:00-07:20 | 13:00-13:20 | Valorisation of Sugar Rich Biomass to High End Fine Chemicals: From Model to Practical Applicable Catalysts<br>Christiaan Tempelman, Rotterdam Mainport Institute, The Netherlands |
| 07:20-07:40 | 13:20-13:40 | CarboChemicals in the Circular Economy<br>Jean-Paul Lange, Shell Global Solutions International, The Netherlands |
| 07:40-08:00 | 14:40-15:00 | Theoretical Considerations on the Electrocatalytic CO2 Reduction Activity of Transition Metal Single-Atom Catalysts<br>Ulla Lassi, University of Oulu, Finland |
| 08:00-08:20 | 18:30-18:50 | Catalytic Thumba Methyl Esters (Biodiesel) Synthesis Using Hydrodynamic Cavitation<br>Abhijeet Dilip Patil, Padmabhooshan Vasantdada Patil Institute of Technology, India |
| 08:20-08:40 | 18:50-19:10 | Transition Metal Based Ternary Hierarchical Metal Sulphide Microspheres as Electrocatalyst for Splitting of Water into Hydrogen and Oxygen Fuels<br>Rohit Srivastava, Pandit Deendayal Petroleum University, India |
| 08:40-09:00 | 19:10-19:30 | Modulating the Redox Conversion between Cu0 and Cu+ on CuxO Decorated ZnOMgO Oxides via *in-situ* Calcination for One-Pot Conversion of CO2 Containing Syngas to Dimethyl ether: Insights from Combined Experimental and DFT Study<br>Kamal Kishore Pant, Indian Institute of Technology Delhi, India |
| 09:00-09:20 | 15:00-15:20 | Mesoporous Aluminosilicate Nanofibers as Acidic Catalytic Support for Selective Phenol Hydrodeoxygenation<br>Sophie Hermans, UC Louvain, Belgium |
| 09:20-09:40 | 15:20-15:40 | Hydrogen Production from Formic Acid Dehydrogenation Catalyzed by Highly Stable Pd-Based Catalysts<br>Miriam Navlani Garcia, University of Alicante, Spain |
| 09:40-10:00 | 15:40-16:00 | Title to be Announced<br>Daniel Puyol, University Rey Juan Carlos, Spain |
| 10:00-10:10 | | **Break** |
| 10:10-10:30 | 15:10-15:30 | Title to be Announced<br>Ruben Ramos Velarde, University of Porto, Portugal |
| 10:30-10:50 | 18:30-18:50 | Microbial Fuel Cell with Enterococcus faecium Biocatalyst<br>Ahmet Erensoy, Firat University, Turkey |
| 10:50-11:10 | 16:50-17:10 | Title to be Announced<br>Natasa Novak Tusar, National Institute of Chemistry, Slovenia |

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|---|---|---|
| 11:10-11:30 | 17:10-17:30 | Power-to-Gas Technology as a Support for Greater Integration of Renewable Energy Sources in the Power System<br>Danko Vidović, Energy Institute Hrvoje Pozar, Croatia |
| 11:30-11:50 | 18:30-18:50 | Impact of Wet-Chemical Synthesis Route on the Nickel State in Ni/BCY15 Proton Conducting pSOFC Anode<br>Dimitrinka Nikolova, Bulgarian Academy of Sciences, Bulgaria |
| 11:50-12:10 | 19:50-20:10 | CoMo Catalysts Supported on Alumina Modified by Mesoporous Zeolites Activity in Hydrodesulfurization of 4,6-DMDBT<br>Aleksey A. Pimerzin, Samara State Technical University, Russia |
| 12:10-12:30 | 14:10-14:30 | Conversion of Co-Mn-Al Hydrotalcites in Highly Active Spinel Catalysts for Peroxide Decomposition<br>Gustavo Doubek, University of Campinas, Brazil |
| 12:30-12:50 | 14:30-14:50 | Nb2O5 Nanotubes as Efficient Platform for Sb2Se3 Immobilization with Catalytic Activity Improvement by Pt Nanoparticles<br>Juliana F. de Brito, Federal University of Sao Carlos, Brazil |
| 12:50-13:10 | 12:50-13:10 | Development of Stable, Low Temperature Methane Oxidation Catalyst (MOC) for Emissions Control of Lean Natural Gas Vehicles<br>Melanie Moses-DeBusk, Oak Ridge National Laboratory, OakRidge, TN, USA |
| **13:10-13:40** | | **Break** |
| 13:40-14:00 | 13:40-14:00 | Title to be Announced<br>Praveen Cheekatamarla, Oak Ridge National Laboratory, OakRidge, TN, USA |
| 14:00-14:20 | 14:00-14:20 | Plasma Generating – Chemical Looping Heterogeneous Porous Binary Catalysts: Quantum Effects in Structure Formation and Plasma Generation<br>Galip Akay, Case Western Reserve University, Cleveland, OH, USA |
| 14:20-14:40 | 14:20-14:40 | Deuterium Enrichments in Hydrocarbons Produced During Ruthenium Catalyzed Fischer-Tropsch Synthesis<br>Buchang Shi, Eastern Kentucky University, Richmond, KY, USA |
| 14:40-15:00 | 12:40-13:00 | Plasma Catalysis for Disassembly of Polymers into Valuable Products<br>Anne M. Gaffney, Idaho National Laboratory, IdahoFalls, ID, USA |
| 15:00-15:20 | 12:00-12:20 | Ni-Ru-MgO Catalyst for Methanation of Producer Gas<br>Robert Cattolica, University of California San Diego, CA, USA |
| 15:20-15:40 | 12:20-12:40 | Lignin Derived Ionic Liquids: Synthesis and Application for Biopolymer Processing<br>Ning Sun, Lawrence Berkeley National Laboratory, Emeryville, CA, USA |
| 15:40-16:00 | 12:40-13:00 | Catalytic Process Design and Development: Highly Efficient and Reversible Hydrogen Generation and Storage Process with Liquid Organic Hydrogen Carriers<br>Ji Su, Lawrence Berkeley National Laboratory, Berkeley, CA, USA |
| 16:00-16:20 | 13:00-13:20 | The Role of Co-Adsorbed Water in Decomposition of Oxygenates<br>Liney Arnadottir, Oregon State University, Corvallis, OR, USA |
| 16:20-16:40 | 16:20-16:40 | Low-dimensional Materials for Energy Storage and Conversion<br>Fei Yao, University at Buffalo, Buffalo, NY, USA |

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| **16:40-17:00** | **15:40-16:00** | Unraveling the Aging Mechanism of Sodium Zincsilicate Catalyst During the Transesterification Reaction Producing Biodiesel<br>Ricardo Rodriguez-Ramirez, Instituto Politecnico Nacional, Mexico |
| **17:00-17:10** | | **Break** |
| **17:10-17:30** | **16:10-16:30** | Potassium Ferrate as Heterogeneous Catalyst for Biodiesel Production Using *Jatropha curcas L.* Oil<br>Adriana Gutierrez-Lopez, Instituto Politecnico Nacional, Mexico |
| **17:30-17:50** | **07:30-07:50**<br>February 23, 2021 | Estimation of CO2 Reduction Potential and Cost of Solid Biomass Fuel Production Process Integrated with a Waste Gasification and Direct Melting System<br>Chihiro Fushimi, Tokyo University of Agriculture and Technology, Japan |
| **17:50-18:10** | **07:50-08:10**<br>February 24, 2021 | Title To be Announced<br>Koichiro Asazawa, Panasonic Corporation, Japan |
| **18:10-18:30** | **08:10-08:30**<br>February 24, 2021 | Development of Zeolite-Based Catalyst for Enhancement the Hydrogen Production from Ammonia Decomposition<br>Mostafa Elshafie, Gifu University, Japan |
| **18:30-18:50** | **08:30-08:50**<br>February 24, 2021 | Plasma Catalysis for Disassembly of Polymers into Valuable Products<br>Oi Lun Helena Li, Pusan National University, South Korea |
| **18:50-19:10** | **08:50-09:10**<br>February 24, 2021 | Ni-Ru-MgO Catalyst for Methanation of Producer Gas<br>Young Su Noh, Korea Institute of Science and Technology (KIST), South Korea |
| **19:10-19:30** | **08:10-08:30**<br>February 24, 2021 | Title to be Announced<br>Kuen-Song Lin, Yuan Ze University, Taiwan |
| **19:30-19:50** | **08:30-08:50**<br>February 24, 2021 | Coal Fly Ash Based Zeolites: A Contemporary Translation of Waste-To-Energy Practice<br>Anjani Ravi Kiran Gollakota, National Yunlin University of Science and Technology, Taiwan |
| **19:50-20:10** | **08:50-09:10**<br>February 24, 2021 | Influence of Porous and Acidic Properties of Aluminosilicate Catalysts on Coke Formation during Lignin Catalytic Pyrolysis<br>Fong-Lee Ng, University of Malaya, Malaysia |
| **20:10-20:30** | **09:10-09:30**<br>February 24, 2021 | Functional Integrated Electromagnetic Interference Shielding in Flexible Micro-Supercapacitors by Cation-Intercalation Typed Ti3C2Tx Mxene<br>Jing Ning, Xidian University, China |
| **20:30-20:50** | **09:30-09:50**<br>February 24, 2021 | Electrocatalytic Upgrading of Biomass Fast Pyrolysis Liquid for Renewable Fuel Precursor Production<br>Jason Lam, City University of Hong Kong, HongKong |
| **20:50-21:10** | **08:50-09:10**<br>February 24, 2021 | Hydrodeoxygenation of Oxygenated Compounds Derived from Pyrolysis of Biomass over Co/TiO2 Catalysts<br>Surachet Hongkailers, Chulalongkorn University, Thailand |

# Session II: Photocatalysis| Electrocatalysis (Parallel Session)

| Meeting Timezone (EST) | Local Time | Chairs: To be Announced |
|---|---|---|
| 6:00-06:20 | 14:00-14:20 | Unprecedented Solar Water Splitting of Dendritic Nanostructured Bi2O3 Films by Combined Oxygen Vacancy Formation and Mo Doping<br>Prabhakarn Arunachalam, King Saud University, Saudi Arabia |
| 6:20-06:40 | 14:20-14:40 | Exploiting the Synergistic Catalytic Effects of CoPi Nanostructures on Zr Doped Highly Ordered TiO2 Nanotubes for Efficient Solar Water Oxidation<br>Mabrook S Amer, King Saud University, Saudi Arabia |
| 6:40-07:00 | 14:40-15:00 | Harvesting Broad Solar Spectrum Via BiVO4 Based Nanoheterostructures For Environmental Remediationon<br>Metwally Madkour, Kuwait University, Kuwait |
| 7:00-7:20 | 14:00-14:20 | Optimization of the Photocatalytic Degradation of Recalcitrant Organic Molecules by Using ZnO Coated Materials<br>Elie Daher, Lebanese University, Lebanon |
| 7:20-7:40 | 13:20-13:40 | Effect of Lithium Doping on Structural, Morphological and Photocatalytic Properties of RE-Doped ZnO<br>Maria Eugenia Rabanal Jimanez, Carlos III University and IAAB, Spain |
| 7:40-8:00 | 12:40-13:00 | From Charge Generation to Hydrogen Evolution Using Polymer<br>Michael Sachs, Imperial College London, UK |
| 8:00-8:20 | 13:00-13:20 | Title to be Announced<br>Kylie A. Vincent, University of Oxford, UK |
| 8:20-8:40 | 14:20-14:40 | Title to be Announced<br>Vincenzo Vaiano, University of Salerno, Italy |
| 8:40-9:00 | 14:40-15:00 | Title to be Announced<br>Giuseppina Iervolino, University of Salerno, Italy |
| 9:00-9:20 | 15:00-15:20 | Title to be Announced<br>Simelys Hernandez, Politecnico di Torino, Italy |
| 9:20-9:30 | | **Break** |
| 9:30-09:50 | 15:30-15:50 | Photocatalytic Transformation of Water Pollutants into Molecular Hydrogen<br>Osama Al-Madanat, Gottfried Wilhelm Leibniz Universität Hannover, Germany |
| 9:50-10:10 | 15:50-16:10 | Title to be Announced<br>Gilles Bourret, University of Salzburg, Germany |
| 10:10-10:30 | 16:10-16:30 | Heterogeneous Photocatalysis of Sulfonamides Using TiO2 and ZnO Photocatalysts – Application of Various Light Sources<br>Tunde Alapi, University of Szeged, Hungary |
| 10:30-10:50 | 16:30-16:50 | Enhancing Photocatalytic Performance by Supporting TiO2 on Stainless Steel Slag: Degradation of Pollutants in Water and Decontamination of Nox<br>Eva Jimenez Relinque, Institute of Construction Science “Eduardo Torroja”. CSIC, Spain |

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|---|---|---|
| 10:50-11:10 | 16:50-17:10 | Photoelectrochemical Behaviour of Nanostructured Anatase Under Different Irradiation Conditions<br>Marta Castellote Armero, Institute of Construction Science “Eduardo Torroja”-CSIC, Spain |
| 11:10-11:30 | 17:10-17:30 | One-Pot Photocatalytic Transformation of Indolines into 3-Thiocyanate Indoles with New Ir(III) Photosensitizers Bearing b-Carbolines<br>Gustavo Espino, Universidad de Castilla, Spain |
| 11:30-11:50 | 18:30-18:50 | Title to be Announced<br>Zsolt Pap, Babes-Bolyai University, Romania |
| 11:50-12:10 | 19:50-20:10 | Electroless/Electrochemical Deposition as Rational Methods for CO Tolerant Catalysts Preparation<br>Kirill Kurdin, Skolkovo Institute of Science and Technology, Russia |
| 12:10-12:30 | 18:10-18:30 | Tin-Modified Titania Photocatalysts with Improved Performance: Sn-TiO2 versus SnO2-TiO2<br>Urska Lavrencic Stangar, University of Ljubljana, Slovenia |
| **12:30-12:40** | | **Break** |
| 12:40-13:00 | 18:40-19:00 | Fiber-Like Structure on Proton Exchange Membrane Created by Simultaneous Magnetron Sputtering and Plasma Etching in Role of a Catalyst Support for Water Electrolyzers<br>Peter Kus, Charles University, Czechia |
| 13:00-13:20 | 13:00-13:20 | Title to be Announced<br>Camilo A. Mesa, Universidad Central Colombia, Colombia |
| 13:20-13:40 | 15:20-15:40 | Visible Light Absorbing Nanorods TiO2 Photocatalytically Deposited onto Flexible Low-Density Polyethylene Films: Characterization and Evaluation of Photocatalytic Activity<br>Julian A. Rengifo-Herrera, Centro de Investigación y Desarrollo, Argentina |
| 13:40-14:00 | 12:40-13:00 | Heterogeneous Gas-Phase Catalysis, Photocatalysis and Electrocatalysis<br>Hoydoo You, Argonne National Laboratory, Lemont, IL, USA |
| 14:00-14:20 | 13:00-13:20 | Transparent Ultramicroelectrodes for Studying Electrocatalytic Reactions Incorporated with Scanning Electrochemical Microscopy<br>Xiao Li, The University of Alabama, Tuscaloosa, AL, USA |
| 14:20-14:40 | 13:20-13:40 | Investigating the Redox Properties of 2D MoS2 Using Photoluminescence Spectroelectrochemistry and Scanning Electrochemical Cell Microscopy<br>Lyndi Strange, The University of Alabama, Tuscaloosa, AL, USA |
| 14:40-15:00 | 14:40-15:00 | Challenges in Clean Energy Nanocatalyst Development<br>Astrid M Mueller, University of Rochester, NY, USA |
| 15:00-15:20 | 15:00-15:20 | Proton Spillover Tuning at Perovskite Surfaces for Non-Faradaic Electrochemical Isomerization Reactions<br>Eugene S. Smotkin, Northeastern University, Boston, MA, USA |
| 15:20-15:40 | 15:20-15:40 | Electrochemistry of Metal-Organic Nanocages for Electrocatalytic Applications<br>Mark Lipke, The State University of New Jersey, Piscataway, NJ, USA |

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| 15:40-16:00 | 15:40-16:00 | Solid-Solution Photocatalysts: New Insights via Percolation Theory<br>Paul A. Maggard, North Carolina State University, Raleigh, NC, USA |
| 16:00-16:10 | | Break |
| 16:10-16:30 | 13:10-13:30 | Ultrafast Intermolecular H-Atom Transfer Reactions Driven by Multipulse Spectroscopy<br>Cody W Schlenker, University of Washington, Seattle, WA, USA |
| 16:30-16:50 | 13:30-13:50 | Explicit Solvent Effects in Electrochemical Reactions<br>Lin-Wang Wang, Lawrence Berkeley National Laboratory, Berkeley, CA, USA |
| 16:50-17:10 | 13:50-14:10 | Transient XUV Studies of Polarons, Interfaces, and Phonons in Photocatalytic Junctions<br>Scott Cushing, Caltech, Pasadena, CA, USA |
| 17:10-17:30 | 14:10-14:30 | Title to be Announced<br>John M Gregoire, Caltech, Pasadena, CA, USA |
| 17:30-17:50 | 14:30-14:50 | Title to be Announced<br>Boniface Fokwa, University of California, Riverside, CA, USA |
| 17:50-18:10 | 17:50-18:10 | Integrating Materials Design and Operando Spectroscopy for the Development of Next Generation CO2 Reduction and Biomass Valorization Catalytic Systems<br>Nikolay Kornienko, Universite de Montreal, Canada |
| 18:10-18:30 | 18:10-18:30 | Electrochemical Systems for CO2 Conversion to C2 Products<br>David Sinton, University of Toronto, Canada |
| 18:30-18:40 | | Break |
| 18:40-19:00 | 10:40-11:00<br>February 24, 2021 | The Essential Role of Electronegativity in Electrocatalysis for Energy Conversion<br>Mengran Li, The University of Queensland, Australia |
| 19:00-19:20 | 11:00-11:20<br>February 24, 2021 | Interactions of Choline Halide Ions with Silver Electrocatalysts for CO2 Reduction<br>Tom Rufford, The University of Queensland, Australia |
| 19:20-19:40 | 11:20-11:40<br>February 24, 2021 | Photocatalytic Filters for Environmental Pollutant Treatment: Design, Fabrication and Application<br>Jinfeng Wang, Deakin University, Australia |
| 19:40-20:00 | 09:40-10:00<br>February 24, 2021 | Evaluation of Oxygen Reduction/Oxygen Evolution Reaction Catalytic Activity of TiN Synthesized by Urea-Glass Method<br>Nataly Carolina Rosero-Navarro, Hokkaido University, Japan |
| 20:00-20:20 | 10:00-10:20<br>February 24, 2021 | Nickel-Based Electrocatalyst Derived from a Nickel Dithioxamide Chelate Polymer for Oxygen Evolution Reaction in Alkaline Solutions<br>Izabela Rzeznicka, Tohoku University, Japan |
| 20:20-20:40 | 10:20-10:40<br>February 24, 2021 | Morphology-Governed Activity of Plasmonic Photocatalysts<br>Ewa Kowalska, Hokkaido University, Japan |
| 20:40-21:00 | 09:40-10:00<br>February 24, 2021 | Electron Transfer Near Metal Surfaces<br>Wenjie Dou, Westlake University, China |
| 21:00-21:20 | 09:00-09:20<br>February 24, 2021 | Heterogeneous Catalysis, Photocatalysis, Simulation of Chemical Processes<br>Pham Thanh Huyen, Hanoi University of Science and Technology, Vietnam |

# Day 3 | February 24, 2021

## Session III: Materials

**Material Sciences | Catalytic Materials & Mechanisms | Polymer Engineering**

| Meeting Timezone (EST) | Local Time | Chairs: To be Announced |
|---|---|---|
| 5:00-5:20 | 13:00-13:20 | Nano-Assembly of SiC Films on Si - A New Met Low-Defect Epitaxial Structures<br>Sergey Kukushkin, IPME RAS, Russia |
| 5:20-5:40 | 13:20-13:40 | Title to be Announced<br>Alexey Tsyganenko, St.Petersburg State University, Russia |
| 5:40-6:00 | 13:40-14:00 | Title to be Announced<br>Olga Russkikh, Ural Federal University, Russia |
| 6:00-6:20 | 16:30-16:50 | Catalytic Activity of Pd- Ni@ DTPA-Iron Oxide in Aqueous Phase Suzuki Coupling Reactions<br>Padmaja Sudhakar Pamidimukkala, University of Baroda, India |
| 6:20-6:40 | 14:20-14:40 | Dry Sliding Wear Behaviour of CeO2-Doped Zirconia<br>Bulent Aktas, Harran University, Turkey |
| 6:40-7:00 | 14:40-15:00 | Title to be Announced<br>Ozgul Gok, Hakkari Universitesi, Turkey |
| 7:00-7:20 | 15:00-15:20 | Polymeric Ionic Liquids of PEI Microgels as Catalyst for Hydrogen Production<br>Nurettin Sahiner, Canakkale Onsekiz Mart University, Turkey |
| 7:20-7:40 | 14:20-14:40 | Title to be Announced<br>Nurit Avraham, Weizmann Institute of Science, Israel |
| 7:40-8:00 | 14:40-15:00 | Chemical and Mechanical Properties of Geopolymers based Incorporated with Cigarette Filters<br>Marianne Saba, University of Balamand, Lebanon |
| **08:00-08:10** | | **Break** |
| 08:10-08:30 | 14:10-14:30 | Exploiting Controlled Reaction-Diffusion Conditions Inside Microfluidic Devices for Materials Synthesis<br>Josep Puigmarti Luis, Institute of Theoretical and Computational Chemistry (IQTC), Spain |
| 08:30-08:50 | 14:30-14:50 | Title to be Announced<br>Maria Eugenia Rabanal Jimenez, Universidad Carlos III de Madrid, Spain |
| 08:50-09:10 | 14:50-15:10 | Computational Simulations on the Amide Bond Formation Catalyzed by Mineral Surfaces<br>Albert Rimola, Universitat Autònoma de Barcelona, Spain |
| 09:10-09:30 | 15:10-15:30 | Future of PCM in Building Applications: Current Problems and Possible Solutions via Nanoconfinement and Template Strategies<br>Felix Marske, Martin-Luther University, Germany |
| 09:30-09:50 | 15:30-15:50 | *In situ* Observations of Supported Nickel Nanoparticles Using Synchrotron X-Ray Diffraction: Insights into Methane Dry Reforming and Carbon Nanotube Growth Mechanisms<br>Albert Gili, Technical University of Berlin, Germany |

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| 09:50-10:10 | 15:50-16:10 | Pursuing Sustainability: Recyclable Organocatalysts Based on Branched Architectures<br>Alena Krupkova, Czech Academy of Sciences, Czech Republic |
| 10:10-10:30 | 16:10-16:30 | Understanding of Cu-Based Supported Catalysts Behavior in Ester Hydrogenolysis<br>Jaroslav Aubrecht, University of Chemistry and Technology Prague, Czech Republic |
| 10:30-10:50 | 16:30-16:50 | Perovskite Photovoltaic Technology on Flexible Substrates<br>Konrad Wojciechowski, Saule Research Institute, Poland |
| **10:50-11:00** | | **Break** |
| 11:00-11:20 | 17:00-17:20 | Polymeric Nanocomposites & Separation and Recovery of Noble Metals<br>Piotr Cyganowski, Wroclaw University of Science and Technology, Poland |
| 11:20-11:40 | 17:20-17:40 | Title to be Announced<br>Marek Wozniak, Lodz University of Technology, Poland |
| 11:40-12:00 | 17:40-18:00 | Structure-Activity Correlation of Platinum Species Supported on Ceria: The Reaction Environment Matters<br>Artiglia Luca, Paul Scherrer Institute, Switzerland |
| 12:00-12:20 | 18:00-18:20 | Learning the Language of Chemical Reactions – Atom by Atom – Using Machine Learning<br>Philippe Schwaller, IBM Research, Switzerland |
| 12:20-12:40 | 18:20-18:40 | Recent Advances in Non-Hydrolytic Sol-Gel Synthesis of Mesoporous Materials for Heterogeneous Catalyst<br>Johan Alauzun, Institut Charles Gerhardt Montpellier, France |
| 12:40-13:00 | 18:40-19:00 | Ruthenium-Based Nanomaterials to Catalyse the Hydrogen Evolution Reaction<br>Karine PHILIPPOT, Universite de Toulouse, France |
| 13:00-13:20 | 19:00-19:20 | Surface or Subsurface? The Case of Hydrogen in Rutile TiO2<br>Calatayud Monica, Sorbonne Universite, France |
| **13:20-13:50** | | **Break** |
| 13:50-14:10 | 19:50-20:10 | Thin and Ultra-Thin Porphyrin Films Used for in Operando Graphite Electrode Protection<br>Gianlorenzo Bussetti, Politecnico di Milano, Italy |
| 14:10-14:30 | 20:10-20:30 | Title to be Announced<br>Juqin Zeng, Istituto Italiano di Tecnologia, Italy |
| 14:30-14:50 | 20:30-20:50 | High Performance Room-Temperature Sputtered Barrier Layer for Standard Solid Oxide Cells<br>Nunzia Coppola, Università di Salerno, Italy |
| 14:50-15:10 | 20:50-21:10 | Characterization of Amorphous Silica Based Materials Using DFT Computational Methods<br>Frederik Tielens, Vrije Universiteit Brussel, Belgium |
| 15:10-15:30 | 15:10-15:30 | Probing 2D Energy Materials with Electrochemical Microreactors<br>Joshua Pondick, Yale University, New Haven, CT, USA |
| 15:30-15:50 | 14:30-14:50 | Title to be Announced<br>Jeffrey Elam, Argonne National Laboratory, Lemont, IL, USA |
| 15:50-16:10 | 15:50-16:10 | Title to be Announced<br>Daniel R Strongin, Temple University, Philadelphia, PA, USA |

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| **16:10-16:30** | **16:10-16:30** | Title to be Announced<br>Samy Madbouly, Penn State Behrend, Erie, PA, USA |
| **16:30-16:50** | **14:30-14:50** | Title to be Announced<br>Dylan Domaille, Colorado School of Mines, Golden, CO, USA |
| **16:50-17:10** | **13:50-14:10** | Title to be Announced<br>William Bowman, University of California, Irvine, CA, USA |
| **17:10-17:20** | **Break** | |
| **17:20-17:40** | **07:20-07:40**<br>February 25, 2021 | Synthesis of Fluoride-Incorporated Polyoxovanadates and Olefin Oxidation<br>Yuji Kikukawa, Kanazawa University, Japan |
| **17:40-18:00** | **07:40-08:00**<br>February 25, 2021 | Design and Synthesis of Metallosupramolecular Catalysts Formed by the Self-Assembly of Functionalized Building Blocks to Mimic Natural Enzymes<br>Shin Aoki, Tokyo University of Science, Japan |
| **18:00-18:20** | **08:00-08:20**<br>February 25, 2021 | Nanoporous Free-standing Flexible Electrodes<br>Radovan Kukobat, Shinshu University, Japan |
| **18:20-18:40** | **08:20-08:40**<br>February 25, 2021 | Title to be Announced<br>Yuki Akagi, The University of Tokyo, Japan |
| **18:40-19:00** | **08:40-09:00**<br>February 25, 2021 | Title to be Announced<br>Sung-Hoon Kim, Silla University, South Korea |
| **19:00-19:20** | **08:00-08:20**<br>February 25, 2021 | CO2 Self-Poisoning and its Mitigation in CuO Catalyzed CO Oxidation: Determining and Speeding Up the Rate-Determining Step<br>Yongsheng Chen, The Chinese University of Hong Kong, Hong Kong |
| **19:20-19:40** | **08:20-08:40**<br>February 25, 2021 | The Chemical Vapour Deposition Growth of Graphene: From Theoretical Calculations to Experimental Synthesis<br>Qinghong Yuan, East China Normal University, China |
| **19:40-20:00** | **08:40-09:00**<br>February 25, 2021 | X-Ray Spectroscopic Study of Atomic and Electronic Structures of Energy Materials<br>Chung-Li Dong, Tamkang University, Taiwan |
| **20:00-20:20** | **08:00-08:20**<br>February 25, 2021 | Synthesis of Value-Added Hydrocarbons via Oxidative Coupling of Methane Over MnTiO3-Na2WO4/SBA-15 Catalyst<br>Anusorn Seubsai, Kasetsart University, Thailand |
| **20:20-20:40** | **06:50-07:10**<br>February 25, 2021 | Effect of Alkali Carbonates Addition on Tri-Doped Ceria: Structure, Microstructure, Ionic Conductivity and Charge Transport Properties for LT-SOFCs Applications<br>Monika Singh, Indian Institute of Technology, Varanasi, India |

# Session IV: Catalysis for Chemical Synthesis (Parallel Session)

| Meeting Timezone (EST) | Local Time | Chairs: To be Announced |
|---|---|---|
| 05:30-05:50 | 19:30-19:50 | Dearomatization and Oxidative Coupling Strategy by Hypervalent Iodine Catalyst in Combination with Green Oxidant<br>Toshifumi Dohi, Ritsumeikan University, Japan |
| 05:50-06:10 | 19:50-20:10 | Efficient Syntheses of Thienoacene Derivatives by Transition Metal-Catalyzed Reactions<br>Koichi Mitsudo, Okayama University, Japan |
| 06:10-06:30 | 20:10-20:30 | Catalytic Asymmetric Nitrene Transfer Reaction<br>Tatsuya Uchida, Kyushu University, Japan |
| 06:30-06:50 | 20:30-20:50 | Nanoparticulate Intermetallic Compound Catalysts Formed on Silica for Hydrosilylation<br>Tomoaki Takayama, Tokyo Institute of Technology, Japan |
| 06:50-07:10 | 20:50-21:10 | Palladium/Carboxylic Acid-catalyzed Alkenylation of Arenes via Carbon-Hydrogen Bond Cleavage<br>Yasunori Minami, National Institute of Advanced Industrial Science and Technology (AIST), Japan |
| 07:10-07:30 | 21:10-21:30 | Title to be Announced<br>Kohei Torikai, Kyushu University, Japan |
| 07:30-07:50 | 21:30-21:50 | Synthesizes Novel Hybrid Visible-Light-Responsive Photocatalysts<br>Hiroaki Tada, Kindai University, Japan |
| 07:50-08:00 | | **Break** |
| 8:00-8:20 | 16:00-16:20 | Noble Metal (Pd, Pt and Rh) Incorporated LaFeO3 Perovskite Catalysts for Oxidative Cracking of n-propane<br>Katabathini Narasimharao, King Abdulaziz University, Saudi Arabia |
| 8:20-8:40 | 16:20-16:40 | New Green Perspective to Dihydropyridine Synthesis Utilizing Modified Heteropoly Acid<br>Mohamed Mokhtar, King Abdulaziz University, Saudi Arabia |
| 8:40-9:00 | 15:40-16:00 | Title to be Announced<br>Lyudmila, University of the Free State, South Africa |
| 9:00-9:20 | 17:00-17:20 | Palladium Nitrosyl Carboxylate Complexes as Catalysts for Oxidative C-H/C-H Coupling of Arenes<br>Oleg Shishilov, Russian Technological University, Russia |
| 9:20-9:40 | 17:20-17:40 | Spark Plasma Sintering for the Synthesis of Nanostructured Carbon Supported Co and Fe Fischer-Tropsch Framework Catalysts<br>Sergei Chernyak, Lomonosov Moscow State University, Russia |
| 9:40-10:00 | 17:40-18:00 | Crystal Chemistry and Topological Features of Micro- and Mesoporous Titanosilicate Catalyst<br>Sergey M. Aksenov, Kola Science Centre, Russia |
| 10:00-10:20 | 20:00-20:20 | Simple Tool for Adding Solid Catalyst without Oxygen and Moisture Contamination<br>Khamid Khodjaniya, Institution of Bioorganic Chemistry, Uzbekistan |
| 10:20-10:30 | | **Break** |

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| **10:30-10:50** | **21:00-21:20** | Phosphine-Free Air-Atable Iridium(III) Complex: An Efficient Catalyst for the a-Alkylation of Arylacetonitriles with Secondary Alcohols<br>Bidraha Bagh, National Institute of Science Education and Research, India |
| **10:50-11:10** | **20:50-21:10** | Selective Hydrogenation of Cinnamaldehyde to Cinnamyl Alcohol Over Palladium/Zirconia in Microwave Protocol<br>Muhammad Sadiq, Bacha Khan University, Pakistan |
| **11:10-11:30** | **21:10-21:30** | Rhodium Complexes in P-C Bond Formation<br>Ana Geer Ramos, Instituto de Sintesis Quimica y Catalisis Homogenea (ISQCH), Spain |
| **11:30-11:50** | **17:30-17:50** | A Flexible Bimetallic Molecular Cage for the Conversion of CO2 into Cyclic Carbonates<br>Valerie Heitz, LSAMM/Institut de Chimie de Strasbourg, France |
| **11:50-12:10** | **17:50-18:10** | A Green Approach to Palladium Catalysed C-C Bond Formation: Heck-Cassar-Sonogashira/Heck/Suzuki Couplings<br>Walter Cabri, University of Bologna, Italy |
| **12:10-12:30** | **18:10-18:30** | Polycyclic Heterocycles by Pd-Catalyzed Processes<br>Raffaella Mancuso, University of Calabria, Italy |
| **12:30-12:50** | **18:30-18:50** | Multicomponent Carbonylative Approaches to Imidazopyridine Derivatives<br>Lucia Veltri, University of Calabria, Italy |
| **12:50-13:10** | **18:50-19:10** | Transition Metal-Catalyzed Reactions: Synthetic Applications<br>Virginie Vidal, PSL Research University, France |
| **13:10-13:30** | **19:10-19:30** | Title to be Announced<br>Torelli Stephane, CEA/CNRS/UGA, France |
| **13:30-14:00** | | **Break** |
| **14:00-14:20** | **19:00-19:20** | Microbubble Interfacial Transformation, Including Catalysis, for CO2 Utilisation<br>William BJ Zimmermane, University of Sheffield, UK |
| **14:20-14:40** | **21:20-21:40** | Microbubble Interfacial Transformation, Including Catalysis, for CO2 Utilisation<br>Nikolaos V. Tzouras, National and Kapodistrian University of Athens, Greece |
| **14:40-15:00** | | Slot Available |
| **15:00-15:20** | | Slot Available |
| **15:20-15:40** | **15:20-15:40** | Enabling Scalable Carbon-Carbon Cross-coupling Chemistry through 3D Printing<br>James K. Ferri, Virginia Commonwealth University, Richmond, VA, USA |
| **15:40-16:00** | **15:40-16:00** | Title to be Announced<br>Dan Xiao, Rensselaer Polytechnic Institute, Troy, NY, USA |
| **16:00-16:20** | **16:00-16:20** | Enzyme-Catalyzed Amine-Functionalization of Poly(Ethylene-glycol)<br>Judit E. Puskas, The Ohio State University, Wooster, OH, USA |
| **16:20-16:40** | **14:20-14:40** | Combining Microbial Biocatalysis with Biocompatible Chemical Catalysis for Single-Pot Production of Industrial Chemicals<br>Dylan W. Domaille, Colorado School of Mines, Golden, CO, USA |
| **16:40-17:00** | **13:40-14:00** | Title to be Announced<br>Eric J. Sorin, California State University, Long Beach, CA, USA |

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| **17:00-17:20** | **14:00-14:20** | Enzyme-Catalyzed Amine-Functionalization of Poly(Ethylene-glycol)<br>Yuan Ping, University of California, Santa Cruz, CA, USA |
| **17:20-17:40** | **08:20-08:40**<br>February 25, 2021 | Facet-Controlled Self-Assembly of ZnO Nanocatalysts – Kinetic Behavior of Benzyl Alcohol Oxidation and Friedel Craft Acylation Reactions<br>Helapiyumi Weerathunga, Queensland University of Technology, Australia |
| **17:40-17:50** | **Break** | |
| **17:50-18:10** | **07:50-08:10**<br>February 25, 2021 | The Effect of Functional Groups on Ordered Mesoporous SiO2 on Direct Synthesis of Hydrogen Peroxide<br>Geun-Ho Han, Korea University, South Korea |
| **18:10-18:30** | **07:10-07:30**<br>February 25, 2021 | Mesoporous Carbons Supported Aggregation-Free Gold Nanoparticles<br>Shangjun Chen, Shanghai Key Laboratory of Rare Earth Functional Materials, China |
| **18:30-18:50** | **07:20-07:40**<br>February 25, 2021 | Copper Nanocomplex with Part-per-Million Catalyst Loadings for Ullmann Reactions at Room Temperature<br>Md Lutfor Rahman, Universiti Malaysia Sabah, Malaysia |
| **18:50-19:10** | **06:50-07:10**<br>February 25, 2021 | Oxidative Coupling of Methane Over Akaline-Earth Metal Oxide-Promoted Lanthanum-Oxide Catalysts<br>Kanticha Jaroenpanon, Kasetsart University, Thailand |
| **19:10-19:30** | **07:10-07:30**<br>February 25, 2021 | Liquid-Phase Selective Hydrogenation of Furfural to Furfuryl Alcohol Over Ferromagnetic Element (Fe, Co, Ni) - Promoted Pt Catalysts Supported on Activated Carbon<br>Sureeporn Saknaphawuth, Chulalongkorn University, Thailand |
| **19:30-19:50** | **07:30-07:50**<br>February 25, 2021 | Hydrogenolysis of Glycerol to Propanediols over ZSM-5-Supported Iridium-Rhenium Catalysts<br>Sarun Chanklang, Kasetsart University, Thailand |

# Day 4 | February 25, 2021

## Session V: Industry

**Nanocatalysis | Nanochemistry | Reaction Engineering | Quantum Chemistry**

| Meeting Timezone (EST) | Local Time | Chairs: To be Announced |
|---|---|---|
| 06:00-06:20 | 21:30-21:50 | Electrochemical Storage Reactions of Hydrogen in Activated Carbon from Phenolic Resin<br>John Andrews, RMIT University, Australia |
| 06:20-06:40 | 21:50-22:10 | Theoretical Considerations on the Electrocatalytic CO2 Reduction Activity of Transition Metal Single-Atom Catalysts<br>Yan Jiao, The University of Adelaide, Australia |
| 06:40-07:00 | 20:40-21:00 | Strategy to Obtain Better Catalysts Using Subnanosized Pt-Alloy Clusters: Origin of High Oxygen Reduction Reaction Activity of Pt12 and Controlling Electronic State Fluctuation<br>Hirotoshi Mori, Chuo University, Japan |
| 07:00-07:20 | 21:00-21:20 | Supported CuPd Bimetallic Nanoalloys as Highly Efficient and Tunable Catalysts for Succinic Acid Hydrogenation<br>Le Dinh Son, Japan Advanced Institute of Science and Technology , Japan |
| 07:20-07:40 | 21:20-21:40 | Microkinetic Modeling for Direct Synthesis of Dimethyl Ether from Syngas over a Hybrid Catalyst<br>Jiyeong Cho, Seoul National University, South Korea |
| 07:40-08:00 | 21:40-22:00 | Atypical Oxygen-bearing Copper Boosts Ethylene Selectivity Toward Electrocatalytic CO2 Reduction<br>Ying Yu, Central China Normal University, China |
| 08:00-08:20 | 16:00-16:20 | Interplay of Biochemical and Biomechanical Reactions and Site-Dependence of Chemical Bonds in Native Bone<br>Andrey A. Pavlychev, Saint Petersburg State University, Russia |
| 08:20-08:40 | 17:20-17:40 | A Simple, Efficient and Bio-Synthesis of Palladium Nanoparticles Using Bael Gum: Application for Reduction of Organic Pollutants and Evaluation of their Antibacterial Activity<br>Kondaiah Seku, University of Technology and Applied Sciences - Shinas, Oman |
| 08:40-08:50 | | **Break** |
| 08:50-09:10 | 14:50-15:10 | Catalytic Activity of DNA on Aggregation Kinetics of Multimodal FHTO-NPs Nanoparticles<br>Elia Maria Grueso Molina, University of Seville, Spain |
| 09:10-09:30 | 17:10-17:30 | Synthesis of Colloidal Solutions of Silver Nanoparticles by *Murraya paniculata* Extracts and their Antimicrobial Activity<br>Irina Antropova, D. Mendeleev University of Chemical Technology, Russia |
| 09:30-09:50 | 15:30-15:50 | Environmentally-Friendly Metal-Based Nanocatalysts: Design and Mechanistic Insight<br>Montserrat Gomez, Universite de Toulouse, France |
| 09:50-10:10 | 15:50-16:10 | Keeping on Renewable Hydrogen Cost: An Analysis on Capex and Opex<br>Javier Brey, Universidad Loyola Andalucia, Spain |

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| **10:10-10:30** | **16:10-16:30** | Nanostructured ceria-titania as efficient photocatalysts for the CO preferential oxidation in H2-rich stream<br>Elisa Moretti, Ca' Foscari University of Venice, Italy |
| **10:30-10:50** | **16:30-16:50** | Nanostructured KIT-6 Materials Functionalized with Sulfonic Groups for Catalytic Purposes<br>Izabela Nowak, Adam Mickiewicz University, Poland |
| **10:50-11:10** | **16:50-17:10** | Polydopamine In The Synthesis Of New Materials For Cancer Therapy<br>Radosław Mrowczyński, Adam Mickiewicz University, Poland |
| **11:10-11:30** | **17:10-17:30** | Towards Understanding the Interface of Polydopamine and Semiconductor NanoMaterials Towards Photocatalytic Water Splitting<br>Emerson Coy, Adam Mickiewicz University, Poland |
| **11:30-11:50** | **17:30-17:50** | To be Announced<br>Neus Domingo, Catalan Institute of Nanoscience and Nanotechnology, Spain |
| **11:50-12:10** | **13:50-14:10** | Bifunctional Oxidase-Peroxidase Inorganic Nanozyme Catalytic Cascade for Wastewater Remediation<br>Herman Sander Man, Federal University of Minas Gerais, Brazil |
| **12:10-12:40** | | **Break** |
| **12:40-13:00** | **11:40-12:00** | Merging Nanotechnology & Synthetic Biology Toward Directed Evolution of Materials for Photocataysis<br>Elena A. Rozhkova, Argonne National Laboratory, Argonne, IL, USA |
| **13:00-13:20** | **12:00-12:20** | Tuning the Morphology of Nanoscale Catalyst to Enable Highly Efficient Chemical Reactions<br>Xiao-Min Lin, Argonne National Laboratory, Argonne, IL, USA |
| **13:20-13:40** | **13:20-13:40** | Bilayer Plasmonic Nano-lattices for Tunable Hydrogen Sensing Platform<br>Tho Nguyen, University of Georgia, Athens, GA, USA |
| **13:40-14:00** | **12:40-13:00** | Characterizing Vanadium Single-Site Catalysts with Computational K-edge XANES<br>Prajay Patel, Argonne National Laboratory, Argonne, IL, USA |
| **14:00-14:20** | **11:00-11:20** | Catalytic Reactions for Enhancement of X-Ray Effects<br>Ting Guo, University of California, Davis, CA, USA |

| Session VI: Simulation & Modeling \| Surface and Colloidal Phenomena \| Organometallics Chemistry | | |
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| **Meeting Timezone (EST)** | **Local Time** | **Chairs: To be Announced** |
| 06:30-06:50 | 22:00-22:20 | Comparison between Parallel and Multi-Serpentine Channel 100 cm2 PEM Fuel Cell<br>Muhammad Arif, RMIT University, Australia |
| 06:50-07:10 | 20:50-21:10 | Improvement of Ion Transport by Deprotonation of Functional Groups in Graphene Oxide Nano-Channel<br>Hae Gon Lee, Yonsei University, South Korea |
| 07:10-07:30 | 21:10-21:30 | Hydrosilylation of Functionalized Alkenes<br>Yumiko Nakajima, National Institute of Advanced Industrial Science and Technology (AIST), Japan |
| 07:30-07:50 | 18:30-18:50 | Optical Studies of Thin Films of Cryocondensed Mixtures of Methanol with Argon or Nitrogen<br>Dmitriy Sokolov, Al-Farabi Kazakh National University, Kazakhstan |
| 07:50-08:10 | 15:50-16:10 | Gel Molselect as an Innovative Method for the Purification of DOTA and DFO Metal Complexes (Ga, Tb) as Analogues of Ga68, Tb161<br>Artem, Mendeleev University of Chemical Technology, Russia |
| 08:10-08:30 | 14:10-14:30 | Effect of the Catalysis on Hydrogenative-ParaHydrogen Induced Polarization (PHIP): Hydrogenation Solvents and Rh(I) Complexes<br>Francesca Reineri, University of Torino, Italy |
| 08:30-08:50 | 14:30-14:50 | Methods for Structural Characterization of Catalytic Processes<br>Rocco Caliandro, Institute of Crystallography, Italy |
| 08:50-09:10 | 14:50-15:10 | Exergo-Economic Analysis of Three Formic Acid Production Processes for the Reuse of Carbon-Dioxide<br>Giorgio Vilardi, University of Rome La Sapienza, Italy |
| **09:10-09:20** | | **Break** |
| 09:20-09:40 | 15:20-15:40 | Tuning Adsorption Energies and Reaction Pathways by Alloying : PdZn Versus Pd for CO2 Reduction to Methanol<br>Emilie Gaudry, Institute Jean Lamour Campus Artem, France |
| 09:40-10:00 | 15:40-16:00 | The Development of Bioinspired Asymmetric Catalysts<br>Srecko Kirin, Ruđer Bosković Institute, Croatia |
| 10:00-10:20 | 16:00-16:20 | Multifaceted Roles of Hydrophilic and Hydrophobized Graphene Oxides in Organic and Photocatalysis: Heterogenized Molecular Catalyst, Flocculant and Promoter Capabilities<br>Tamas Szabo, University of Szeged, Hungary |
| 10:20-10:40 | 16:20-16:40 | Solvation Effects on the Structure and Reactivity of Co3O4 (001) Surfaces: A Molecular Dynamics Study<br>Stephane Kenmoe, University of Duisburg-Essen, Germany |
| 10:40-11:00 | 10:40-11:00 | Antifreeze Proteins: A Team Effort to Accelerate and Inhibit Ice Growth<br>Ran Drori, Yeshiva University, New York, NY, USA |
| 11:00-11:20 | 11:00-11:20 | A Modular Toolbox Based on Iridium, Rhodium and Amino Acids for Homogeneous Asymmetric Transfer Hydrogenation<br>Joseph S. Merola, Virginia Tech, Blacksburg, VA, USA |
| 11:20-11:40 | 11:20-11:40 | Balancing Multiple Orthogonal Functions Simultaneously on a Single Surface<br>Timothy Lawton, US Army - CCDC Soldier Center, Natick, MA, USA |
| 11:40-12:00 | 10:40-11:00 | Urine Foam Fractionation<br>Arturo A. Garcia-Figueroa, Universidad Nacional Autónoma de Mexico, Mexico |
| 12:50-13:10 | 10:50-11:10 | Ligand Effects on Decarbonylation of Palladium-Acyl Complexes<br>Bess Vlaisavljevich, University of South Dakota, Vermillion, SD, USA |

# Day 5 | February 26, 2021

| Session VII: Environmental Catalysis \| Catalysis and Pyrolysis \| Catalysis and Zeolites \| Enzymes & Biocatalysts | | |
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| **Meeting Timezone (EST)** | **Local Time** | **Chairs: To be Announced** |
| 06:40-07:00 | 17:10-17:30 | From Laboratory to Industrial Scale: A Scaleup Framework for Biocatalysis<br>Pravin Kumar R, Kcat Enzymatic Private Limited, India |
| 07:00-07:20 | 21:00-21:20 | Three-Way Catalytic Performance and Chemical State of Cu Added Al2O3 Catalysts<br>Masatomo Hattori, Nagoya University, Japan |
| 07:20-07:40 | 21:20-21:40 | Microbial Fuel Cell with Enterococcus faecium Biocatalyst<br>Rahat Javaid, National Institute of Advanced Industrial Science and Technology, Japan |
| 07:40-08:00 | 21:40-22:00 | Improvement of Ion Transport by Deprotonation of Functional Groups in Graphene Oxide Nano-Channel<br>Haegon Lee, Yonsei University, South Korea |
| 08:00-08:20 | 21:00-21:20 | PVA-Metal Porphyrin Hydrogel Confinement for Controlled Photocatalytic Oxidation of Sulfides in Water with Micro-Aeration to Elemental Sulfur by Visible Light<br>Lau Chun Yin, Hong Kong Polytechnic University, Hong Kong |
| 08:20-08:40 | 16:20-16:40 | Synthesis of N-Doped Carbon Nanofibers Over Ni-M Alloys Prepared via Mechanochemical Alloying Approach<br>Ilya Mishakov, Novosibirsk State University, Russia |
| 08:40-09:00 | 16:40-17:00 | Obtaining and Using Nanomaterials for Displacing Oil from a Porous Medium<br>Boris Ezdin, Novosibirsk State University, Russia |
| 09:00-09:20 | 16:00-16:20 | Ozone Initiated Catalytic Oxidation of 1,2-Dichlorobenzene Using Manganese Loaded Metal Oxides<br>V.S.R. Rajasekhar Pullabhotla, University of Zululand, South Africa |
| 09:20-09:40 | 21:20-21:40 | One-Pot Conversion of Furfural to ɣ-Valerolactone oOver Co- and Pt-Doped ZSM-5 Catalysts<br>Weerachon Tolek, Chulalongkorn University, Thailand |
| 09:40-10:00 | 20:10-20:30 | Mesozeolite BEA Catalyzed Multicomponent Reactions for Green Synthesis of Biologically Active Heterocyclic Scaffolds<br>Kalpana Maheria, S. V. National Institute of Technology, India |
| **10:00-10:10** | | **Break** |
| 10:10-10:30 | 20:40-21:00 | Optimization of the Sonocatalytic Degradation of Tetracycline with Cu-Doped TiO2 Catalyst Using Response Surface Methodology<br>Amritanshu Shriwastav, Indian Institute of Technology Bombay, India |
| 10:30-10:50 | 21:00-21:20 | Biodiesel Production from Indigenous Non-Edible Feedstocks Using Immobilized *Pseudomonas cepacia* Lipase<br>Bhawna Verma, Banaras Hindu University, India |
| 10:50-11:10 | 21:20-21:40 | Multifunctional After Treatment System for NOx Adsorption and Reduction: Development and Mechanistic Insights<br>Prateek Khatri, Indian Institute Of Technology Delhi, India |
| 11:10-11:30 | 19:10-19:30 | Activity of Nickel-Based Catalysts for Dry Reforming of Biogas in the Presence of H2S: Effect of Manganese Incorporation<br>Hale Akansu, Gazi University, Turkey |

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| 11:30-11:50 | 17:30-17:50 | Efficient Conversion of Xylose to Glycolic Acid Over Zn3V2O8 Mixed Oxide Catalyst in Water<br>Abdelhak Kherbeche, Sidi Mohammed Ben Abdellah University, Morocco |
| 11:50-12:10 | 17:50-18:10 | Influence of Water Vapor on the Behavior of a CuO/SBA-15 Type SOx Adsorbent in a Cyclic Flue Gas Desulphurization Process<br>Gregory Guicheney, University de Haute Alsace, France |
| 12:10-12:30 | 18:10-18:30 | Green Methods in the Synthesis of Organosilicon and Organoboron Compounds via Catalytic Hydrometallation and Coupling Reactions<br>Jedrzej Walkowiak, Adam Mickiewicz University in Poznan, Poland |
| 12:30-12:50 | 18:30-18:50 | Increasing the Photodegradation Efficiency of ZnWO4 by Synthesizing a Bi2WO6/ZnWO4 Composite Photocatalyst<br>Praveen Kumar, University of Ljubljana, Slovenia |
| **12:50-13:20** | | **Break** |
| 13:20-13:40 | 20:20-20:40 | Porous Geopolymers for Catalytic Water Treatment Applications<br>Anne Heponiemi, University of Oulu, Finland |
| 13:40-14:00 | 19:40-20:00 | Polystyrene/Fe3O4/MWCNTs New Nanocomposite for Toluene Removal from Water<br>Thamer Adnan Abdullah, University of Pannonia, Hungary |
| 14:00-14:20 | 20:00-20:20 | Synthesis of Hierarchical Zeolites Containing Niobium and their Application in Epoxidation of Cyclohexene<br>Agnieszka Feliczak-Guzik, Adam Mickiewicz University, Poland |
| 14:20-14:40 | 20:20-20:40 | The Role of Tyr/Trp Redox Pathways in Biocatalytic Oxygen Reduction – A Case Study of *S. Coelicolor* Laccase<br>Patrycja Kielb, University of Potsdamty, Germany |
| 14:40-15:00 | 19:40-20:00 | The Application of TiO2 Nanomaterials for the Photocatalytic Removal of Selected Pharmaceuticals from Industrial Waste Streams<br>Kieran Nolan, Dublin City University, Ireland |
| 15:00-15:20 | 21:00-21:20 | Influence of Porous and Acidic Properties of Aluminosilicate Catalysts on Coke Formation During Lignin Catalytic Pyrolysis<br>Hanmin Yang, KTH, Sweden |
| 15:20-15:40 | 17:20-17:40 | Mechanistic Investigation of the Dehydration of Lactic Acid on Alkali-Exchange Zeolites through an *in-situ* FT-IR<br>Maria Angelica Perillo, National University of Cordoba, Argentina |
| 15:40-16:00 | 12:40-13:00 | Cu-Al-Oxo Clusters on Mordenite: Combined Study of Ab-Initio Molecular Dynamics, Ensemble Averaged XAS Simulations, and Experiments<br><br>Mal Soon Lee, Pacific Northwest National Laboratory, Richland, WA, USA |
| **16:00-16:10** | | **Break** |
| 16:10-16:30 | 16:10-16:30 | Interpretable Machine Learning Model for Predicting TiO2-Catalyzed Photo-degradation Rate of Water Contaminants<br>Xiong (Bill) Yu, Case Western Reserve University, Cleveland, OH, USA |
| 16:30-16:50 | 16:30-16:50 | Title to be Announced<br>Fudong Liu, University of Central Florida, Orlando, FL, USA |
| 16:50-17:10 | 16:50-17:10 | A Catalase Mimic with Exceptional Activity and Selectivity<br>Andrew G. Tennyson, Clemson University, Clemson, SC, USA |

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| **17:10-17:30** | **16:10-16:30** | Deconstructing and Upcycling of Plastic Solid Wastes by Catalytic Microwave-Assisted Pyrolysis System with Focus on High Quality Naphtha Production<br>Roger Ruan, University of Minnesota, Minneapolis, MN, USA |
| **17:30-17:50** | **16:30-16:50** | Biocatalytic Protein Modification Using Farnesyltransferase<br>Mark D. Distefano, University of Minnesota, Minneapolis, MN, USA |
| **17:50-18:10** | **15:40-16:00** | Oxidative Water Treatment Using Persulfates: Kinetic Modeling and Galvanic Oxidation Processes<br>Huichun (Judy) Zhang, Case Western Reserve University, Cleveland, OH, USA |
| **18:10-18:30** | **18:10-18:30** | Nanozyme Scavenging ROS for Prevention of Pathological Alpha-Synuclein Transmission in Parkinson's Disease<br>Xiaobo Mao, Johns Hopkins University School of Medicine, Baltimore, MD, USA |

**Last minute changes due to functional, private, or organizational needs can be necessary.**
**Program is subject to change**