

Catalysis and Reaction Engineering Division

Held at the 2023 AIChE Annual Meeting

Orlando, Florida, USA
5-10 November 2023

ISBN: 978-1-7138-9296-0

Printed from e-media with permission by:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571



Some format issues inherent in the e-media version may also appear in this print version.

Copyright© (2023) by AIChE
All rights reserved.

Printed with permission by Curran Associates, Inc. (2024)

For permission requests, please contact AIChE
at the address below.

AIChE
120 Wall Street, FL 23
New York, NY 10005-4020

Phone: (800) 242-4363
Fax: (203) 775-5177

www.aiche.org

Additional copies of this publication are available from:

Curran Associates, Inc.
57 Morehouse Lane
Red Hook, NY 12571 USA
Phone: 845-758-0400
Fax: 845-758-2633
Email: curran@proceedings.com
Web: www.proceedings.com

TABLE OF CONTENTS

IN HONOR OF KLAUS JENSEN'S 70TH BIRTHDAY (INVITED TALKS)

419a Reframing Computing and Artificial Intelligence: Based on Principles from Statistical/Quantum Physics, Chemistry, and Information Theory	1
<i>Sadasivan Shankar</i>	
419b Making Molecules and Materials in Fluidic Factories	2
<i>Saif Khan</i>	
419c New Avenues in Data-Centric Microreaction Engineering for a Sustainable Future.....	3
<i>Ryan Hartman</i>	
419d Development and Scale-up of Flow Chemical Syntheses for Drug Substance Manufacturing.....	4
<i>Jonathan McMullen</i>	
419e Ultrasound As a Process Intensification Tool in Small-Scale Reactors	5
<i>Simon Kuhn</i>	
419f Self-Driving Fluidic Labs: Autonomous Experimentation in Flow to Accelerate Materials and Molecular Discovery	6
<i>Milad Abolhasani</i>	
419g Liquid Water-Tolerant Solid Bronsted Acid Catalysts Based on Sulfonic Acid-Functionalized Zeolite Beta	7
<i>Marcella Lusardi</i>	
419h Experimental Design: From Iterative Reaction Optimization to Route Planning with Literature Data.....	8
<i>Connor Coley</i>	

IN HONOR OF THE 2021 R.H. WILHELM AWARD WINNER I (INVITED TALKS)

293a New Facilitated Transport Membrane and Process for CO ₂ Capture from Flue Gas.....	9
<i>Yang Han, Yutong Yang, Babul Prasad, W.S. Winston Ho</i>	
293b Interfacial Oriented Assembly of Hierarchical-Pore Functional Mesoporous Materials from Monomicelles	10
<i>Dongyuan Zhao</i>	
293c Platinum Group Metal-Free Catalysts for Electrochemical Energy Conversion	11
<i>Piotr Zelenay</i>	
293d Heterogeneous Molecular Catalysts for Electrocatalytic Applications.....	12
<i>Xin Wang</i>	
293e Controlling Interfacial Electron and Atom Transfer Reactions.....	13
<i>Karthish Manthiram</i>	
293f Towards Highly Active Hydrogen Oxidation Reaction Electrocatalysts in Alkaline	14
<i>Zhongbin Zhuang</i>	

293g Nickel-Based Anode Catalysts for Efficient and Affordable Hydroxide Exchange Membrane Fuel Cells.....	15
<i>Min-Rui Gao</i>	
293h Li(Ni,Co,Mn)O ₂ Nanoparticles for Oxygen Electrocatalyst.....	16
<i>Hongmei Luo</i>	
293i Mathematical Modeling of Redox-Mediated Processes in Electrochemical Systems	17
<i>Nicholas Matteucci II, Fikile Brushett</i>	

IN HONOR OF THE 2021 R.H. WILHELM AWARD WINNER II (INVITED TALKS)

345a Challenges in the Simulation of the Electrochemical Reduction of CO ₂	18
<i>Alexis T. Bell</i>	
345b Superstructured Materials for Energy Conversion and Storage.....	19
<i>Yun Hang Hu</i>	
345c Electrocatalytic Oxidative Dehydrogenation of Biorenewable Aldehydes over Cu-Based Catalysts for Bipolar Hydrogen Production	20
<i>Wenzhen Li</i>	
345d Micro-Supercapacitors Based-on Mxene Quantum Dots with Ultra-High Rate Capability and Fast Frequency Responsibility.....	21
<i>Aiping Yu</i>	
345e Materials, Integration, and Durability Challenges in Low Temperature Electrolysis	22
<i>Shaun Alia</i>	
345g Applying Atomic-Scale Surface Modification to Catalysis and Energy Storage.....	23
<i>Stacey F. Bent</i>	
345h Rechargeable Zinc-Air Battery	24
<i>Zhongwei Chen</i>	

PIONEERS OF CATALYSIS AND REACTION ENGINEERING (INVITED TALKS)

493a Computationally Tackling Interfacial Chemistry of Compounds Materials	25
<i>Aleksandra Vojvodic</i>	
493b “Advanced” Materials Characterization of Catalysts at BASF	26
<i>Robert M. Palomino, Ahmad Moini, Eduard Kunkes, Ke-Bin Low, Florian Waltz, Chunxin Ji, Thomas Schmitz, Ivan Petrovic</i>	
493c Toluene Alkylation with Light Alkenes on Acidic Mordenite: The Effects of Acid Size Locations and Confinements on Reaction Mechanisms	27
<i>Stephanie Kwon</i>	
493d Fundamental Insights into Chemical Recycling of Polymer Mixtures	28
<i>Hilal Ezgi Toraman</i>	
493e Pioneering a New Paradigm in Exchange-Correlation Functional Design	29
<i>Andrew Medford, Xiangyun Lei, Sushree Jagriti Sahoo</i>	

**MID CAREER RESEARCHERS IN CATALYSIS AND REACTION ENGINEERING
RECOGNITION SYMPOSIUM (INVITED TALKS)**

470a High-Temperature Electrolysis over Perovskites : The Role of Exsolution of Metal Nano- Particles	30
<i>Umit Ozkan, Dhruva Jyoti Deka, Seval Gunduz, Jaesung Kim</i>	
470b An Electrochemical Engineering Journey Towards Sustainable Nylon Precursors	31
<i>Miguel Modestino</i>	
470d Coupling CO ₂ Capture and Electrochemical Reduction Using Azolide Ionic Liquids	32
<i>Jon-Marc McGregor, Louise M. Cañada, Joaquin Resasco, Joan Brennecke</i>	
470e Electrochemical Routes for Nutrient Recovery from Sludge.....	33
<i>Jedidian A. Adjei, Ehsan Abbasi, Maasoomah (Masi) Jafari, Gerardine G. Botte</i>	
470f Understanding Fluid Structure and Properties of Concentrated Hydrogen Bonded Electrolytes (CoHBES) and Their Interaction in a Flow Battery	34
<i>Robert F. Savinell, Burcu Gurkan</i>	
470g Electrochemical Reaction Engineering for Green Chemistry and Energy: Electrocatalysis and Electrolytes	35
<i>Elizabeth Biddinger</i>	

IN HONOR OF THE 2022 R.H. WILHELM AWARD WINNER I (INVITED TALKS)

127a In Honor of Phillip E. Savage: Molecular-Level Kinetic Modeling in Thermochemical Conversions	36
<i>Michael Klein</i>	
127b Glycerol-Derived Compounds As Bio-Based Solvents for Organosolv Pulping of Lignocellulosic Biomass	37
<i>James D. Sheehan, Jason Bara, Jayna M. Enguita</i>	
127c Thermo-Catalytic Approaches for the Conversion of Biomass into Hydrocarbons	38
<i>Fernando Resende</i>	
127d Effects of Lewis Acid Strength on Methanol Dehydration in Microporous Solid Acids.....	39
<i>Musa Mohammed, Gunnar Sly, Gina Noh</i>	
127e Beyond the Active Site - Controlling the Local Chemical Environment of Active Sites to Achieve Improved Catalytic Performance.....	40
<i>Suljo Linic</i>	
127f Ethane Dehydrogenation Using Solar Energy.....	41
<i>Abhaya K. Datye, Andrew T. DeLaRiva, Christopher Riley, Jeffrey Weissman, Andre DeCarmine, Alexander Brown, Erik Spoerke</i>	
127g Why Don't You Go Figure It out: A Nudge Towards a Career in Sustainability Analysis.....	42
<i>Jennifer Dunn</i>	

IN HONOR OF THE 2022 R.H. WILHELM AWARD WINNER II (INVITED TALKS)

215a Reflections on 40 Years in Chemical Reaction Engineering.....	43
<i>Phillip Savage</i>	
215b Advancing Towards Scale-up, Developments in Hydrothermal Liquefaction of Biomass at Pacific Northwest National Laboratory	44
<i>Peter Valdez, Michael R. Thorson, Andrew J. Schmidt</i>	
215c Molecular and Mechanistic Modeling of Heterogeneous Catalysis in Supercritical Fluids	45
<i>Kenneth Benjamin</i>	
215d Insights into Co-Pyrolysis of Plastics through Experiments and Kinetic Modeling.....	46
<i>Hilal Ezgi Toraman</i>	
215e Integration and Digitalization in the Manufacturing of Therapeutic Proteins.....	47
<i>Massimo Morbidelli, Alberto Cavazzini</i>	

IN HONOR OF RAY GORTE'S ACHIEVEMENTS (INVITED TALKS)

439a Enzyme Driven Synthesis of High-Performance Heterostructured Photocatalysts.....	48
<i>Steven McIntosh</i>	
439c Structure-Activity Relationships for Zirconia-Based Catalysts	49
<i>Mengjie Fan, John Vohs</i>	
439d A “Cerious” Collaboration on Supported Metals and Much More	50
<i>Paolo Fornasiero</i>	
439e Lessons Learned and Applied from Gorte's Mentorship.....	51
<i>David Parrillo</i>	
439f High Resolution Atomic Force Microscopy Study of an Immobilized Molecular CO ₂ Reduction Electrocatalyst.....	52
<i>Xinzhe Wang, Percy Zahl, Hailiang Wang, Udo D. Schwarz, Eric Altman</i>	
439g Fabrication of Nano-Structured Catalysts and Catalyst Supports By ALD	53
<i>Raymond Gorte</i>	

IN MEMORIAM OF MARIA FLYTZANI-STEPHANOPOULOS (INVITED TALKS)

366a Self-Healing Catalysts Via Atom Trapping.....	54
<i>Abhaya K. Datye, Stephen Porter, Arnab Ghosh, Ryan Alcalá, Eric J. Peterson, Hien N. Pham, Deepak Kunwar, Chase Thompson, Andrew T. DeLaRiva, Adrian Brearley, John Watt, David P. Dean, Jeffrey T. Miller, Chih-Han Liu, Eleni Kyriakidou</i>	
366b Well-Defined Inverse Oxide/Metal Systems As Active and Selective Heterogeneous Catalysts	55
<i>Jose Rodriguez</i>	
366c Novel Single-Site Catalysts for the Dehydrogenation of Light Alkanes.....	56
<i>Alexis T. Bell</i>	

366e A Decade-Long Quest into Understanding and Developing Novel Single-Atom Alloy Catalysts	57
<i>Michail Stamatakis</i>	

CATALYST DESIGN, SYNTHESIS, AND CHARACTERIZATION I: DESIGN OF CATALYTIC NANOPARTICLE ALLOYS

581a Formation of Dilute Ti-Cu(111) Surface Alloys and Their High Selectivity Toward Ethanol Deoxygenation to Ethylene	58
<i>Junjie Shi, Hio Tong Ngan, Cameron Owen, Vikram Mehar, Siyu Qin, Philippe Sautet, Jason Weaver</i>	
581c Synthesis and Performance of Encapsulated Au/Pd Nanoparticles in Zeolites for Oxidation Catalysis	59
<i>Cole Hullfish, Michele Sarazen</i>	
581d Computational Design of Alloy Catalysts for Propane Conversion.....	60
<i>Sarah Stratton, Matthew Montemore</i>	
581e Structural Evolution of Au-Pd Single Atom Alloy Catalysts for H ₂ O ₂ Synthesis	61
<i>Conor Waldt, Suchi Vijayaraghavan, David Flaherty, Ayman M. Karim, David Hibbitts</i>	
581f Controlling the Performance of Cu/SiO ₂ Catalysts for Methyl Acetate Hydrogenation By the Introduction of Dilute Quantities of Pt.....	62
<i>Damilola Akinneye, J. Will Medlin</i>	
581g Strong Metal-Support Interaction Effects on PdAg Alloy Nanoparticles: A Promising Approach for Acetylene Semi-Hydrogenation	63
<i>Zihao Yan, Huiyuan Zhu</i>	
581h Development of Methods for Precise, Multifactor Tuning of Shell Thickness and Pore Diameter of Silica-Encapsulated Gold Core-Shell Nanoparticles	64
<i>Ellis Hammond-Pereira, Steven Saunders</i>	

CATALYSIS ON LOW DIMENSIONAL MATERIALS

561a Discovering Single Site and Single Atom Catalysts with High-Throughput Computational Screening	66
<i>Heather Kulik</i>	
561b Effect of Geometry, Spin, and Applied Potential in Oxygen Evolution and Reduction Reactions for Atomically Disperse Carbon-Based Electrocatalysts	67
<i>Md Delowar Hossain, Michal Bajdich</i>	
561c Oxides Supported Transition Metal Single Atoms for Oxygen Electrocatalysis	68
<i>G. T. Kasun Kalhara Gunasooriya</i>	
561d Activity Descriptor Identification of Edge-Hosted Fe-N ₃ Sites for the Catalytic Transfer Hydrogenation	69
<i>Piaoping Yang, Stavros Caratzoulas, Jiang Li, Dionisios Vlachos</i>	
561e Predicting the Adhesion Energies and Sinter Resistance of Metal Films on Carbide and Nitride Supports	70
<i>Lavie Rekhi, Kah Meng Yam, Pranav Roy, Tej Choksi</i>	

561f Designing Two Dimensional Materials for Oxygen Electrocatalysis.....	71
<i>Samira Siahrostami</i>	

MICROPOROUS AND MESOPOROUS MATERIALS I: MATERIALS DESIGN

689a Thermodynamics of Al Substitution in CHA with and without Organic Structure-Directing Agents.....	72
<i>Alexander Hoffman, Mingrou Xie, Cecilia Paris, Manuel Moliner, Rafael Gomez-Bombarelli</i>	
689b Controlling Intrinsic Defects in Hierarchical Zeolite ZSM-5 Catalysts and Their Impact on Methanol to Hydrocarbons	74
<i>Kumari Shilpa, Michael Tsapatsis, Jeffrey Rimer</i>	
689c Influence of N,N,N-Trimethyl-1-Adamantyl Ammonium on Al and Defect Siting Energetics and Implications for Accessible Si/Al Ratios in CHA.....	75
<i>Xuyao Gao, Craig Waitt, Ahmad Moini, Rajamani Gounder, William Schneider</i>	
689d A Computational Roadmap for the De Novo Design of Organic Structure Directing Agents for Zeolite Synthesis	76
<i>Mingrou Xie, Daniel Schwalbe-Koda, Omar Santiago Reyes, Alexander Hoffman, Cecilia Paris, Manuel Moliner, Rafael Gomez-Bombarelli</i>	
689e Quantifying the Kinetics of Framework Dealumination during Hydrothermal Aging of Proton-Form CHA Zeolites	77
<i>Tania Class Martinez, Subramanian Prasad, Ahmad Moini, Rajamani Gounder</i>	
689f Cooperative Catalytic Site Evolution upon Catalyst Recycling for Heterogeneous Aminosilica Materials in the Aldol Reaction and Condensation	78
<i>Jee-Yee Chen, Nicholas Brunelli</i>	
689g Identification of Multinuclear Copper Active Sites for NO Oxidation over Cu-SSZ-13.....	80
<i>Ishant Khurana, Jonatan D. Albarracin Caballero, Arthur Shih</i>	
689h Base Enhanced Activation of Phosphorous-Containing Zeolites	81
<i>Han Chen, Jason Gulbinski, Choongsze Lee, Tarnuma Tabassum, Michael Tsapatsis, Wei Fan, Susannah L. Scott, Dionisios Vlachos, Stavros Caratzoulas, Omar Abdelrahman</i>	

NEW DEVELOPMENTS IN COMPUTATIONAL CATALYSIS I: PHYSICS-BASED METHODS

695a Beyond Conventional Transition State Theory in Catalysis: Applications of Matrix Completion	82
<i>Selin Bac, Jeongmin Chae, Urbashi Mitra, Shaama Mallikarjun Sharada</i>	
695b CO ₂ Reduction on Copper: Mechanistic Analysis from Accurate Electronic Structure Methods.....	83
<i>Qing Zhao</i>	
695c Multi-Scale Modeling of Electrocatalytic Processes within the Electrochemical Double Layer.....	84
<i>Andrew Wong, Bolton Tran, Derek Zhu, Scott T. Milner, Michael Janik</i>	
695d Development of Non-Empirical Tight Binding Theory for Efficient Quantum Chemical Calculations	86
<i>Alanna Leung, Alexander Mironenko</i>	

695f Boosting the Accuracy of Formation Enthalpies of Adsorbates from DFT through Error Cancellation.....	87
<i>Bjarne Kreitz, C Franklin Goldsmith</i>	

695g Fast and Accurate Assessment of Electronic Structure Changes of Nanocatalysts upon Alloying and Adsorption	88
<i>Filippo Balzaretti</i>	

NITROGEN CHEMISTRY I: NITROGEN ELECTROCHEMISTRY

697a Strategies for Steering Selectivity during Catalytic Nitrate Reduction.....	89
<i>Yu Chen, Thomas Senftle</i>	

697b Lithium Mediated Electrochemical Synthesis of Ammonia at High Pressures	90
<i>Ishita Goyal, Nishithan Balaji Chidambara Kani, Meenesh R Singh</i>	

697c Carbon-Mediated Photocatalytic Nitrogen Fixation on Titania	91
<i>Po-Wei Huang, Yu-Hsuan Liu, Tijana Rajh, Nianhan Tian, Giada Innocenti, Carsten Sievers, Andrew Medford, Marta Hatzell</i>	

697d Elucidating the Mechanisms of Electrochemical Nitrogen Oxidation Reactions (NORs) on Metal Oxides	92
<i>Alexandra Zagalskaya, Sneha Akhade, Jeremy T. Feaster</i>	

697e First-Principles Design of Nitrogen Reduction Catalysts: Taking Inspiration from Nature	93
<i>Lakshay Dheer, Frank Abild-Pedersen, Michal Bajdich</i>	

697f Modeling Acidic Nitrate Reduction on Early Transition Metal Surfaces	94
<i>Michael Tang, Joakim Halldin Stenlid, Jinyu Guo, Elizabeth Corson, Matthew J. Liu, William Tarpeh, Frank Abild-Pedersen</i>	

697g Unveiling the Mechanism of Green Ammonia Production on the Ti ₂ N Nitride Mxene Via in-Situ Spectroelectrochemistry	95
<i>Denis Johnson, Ray Yoo, Abdoulaye Djire</i>	

LOW CARBON HYDROGEN GENERATION

688a High Throughput Discovery of Ternary Cu-Fe-Ru Alloy Catalysts for Photo-Driven Hydrogen Production	96
<i>Maya Bhat, Zoe Simon, Savannah Talledo, Riti Sen, Jacob Smith, Stefan Bernhard, Jill E. Millstone, John Kitchen</i>	

688b A Continuous Process for the Thermochemical Production of Green Hydrogen.....	97
<i>Casper Brady, Elizabeth G. Mahoney, Peter Chea, Mark Davis</i>	

688c The Dehydrogenation of Methyl Cyclohexane on Pt Nanoclusters: Insights from a First Principles Microkinetic Model.	98
<i>Chuhong Lin, Voon Huey Lim, Xin Zhao, Rong Xu, Tej Choksi</i>	

688e A Microkinetic Framework to Understand the Promoting Role of Ba on Co-Ce Catalyst for Hydrogen Production Via Ammonia Decomposition	100
<i>Natalia Realpe, Gontzal Lezcano, Shekhar Kulkarni, Salvador Sayas, Natalia Morlanes, Jose Cerillo, Mohammad Rakib, Ragad F. Aldilajjan, Sai P. Katikaneni, Bandar Solami, Jorge Gascon, Pedro Castano</i>	

688f Reactor Design Considerations for the Efficient Hydrogen Production through Combined Natural and Artificial Light-Driven Photocatalytic Water Splitting	101
<i>Ahmed Abbas, Shohda Makki, Konstantinos Kakosimos</i>	
688g Green H ₂ Production through Biochar Advanced Water Electrolysis.....	102
<i>Rohit Chauhan, Nishithan Balaji Chidambara Kani, Meenesh R Singh</i>	
688h Exploring the Kinetic and Mechanism of Methane Decomposition to CO _x -Free Hydrogen and Carbon Nanotubes Using Ni-Mo/MgO As a Catalyst	103
<i>Laura A. Gomez, Caleb Q. Bavluka, Phuong Nguyen Thi, Ismaeel I. Alalq, Steven Crossley, Daniel E. Resasco</i>	

INTERSECTION BETWEEN THERMAL AND ELECTROCATALYSIS

687a Mechanistic Insights into Mediated Chemical and Electrochemical Routes for O ₂ reduction over Metal and Nitrogen-Doped Carbon (M-N-C) Catalysts	104
<i>Mayank Tanwar, Jason Bates, Shannon S. Stahl, Matthew Neurock</i>	
Thermal-Electro-Synthesis of Ammonia over Molybdenum Oxynitride at 250°C	105
<i>Arthur Shih, Dylan Bardgett, Elise Goldfine, Louis Wang, Grace Xiong, Paul Chery, Tiffany Miao, Sarah Bogan, Sossina M. Haile</i>	
687b Leveraging Thermochemical Reaction Steps in the Electrocatalytic Activation of C(sp ³)-H Bonds.....	106
<i>Christine Lucky, Lee Fuller, Marcel Schreier</i>	
687c Design Strategies for Efficient Perovskite Oxide Electrocatalysts: Extending Concepts from Thermal Catalysis to Describe Their Electrocatalytic Performance	107
<i>Samji Samira, Eranda Nikolla</i>	
687d Deep Learning Boosted Field-Driven Catalysis	108
<i>Mingyu Wan, Han Yue, Jaime Notarangelo, Hongfu Liu, Fanglin Che</i>	
687e The Preferential Electrochemical Activity of Au and Pd Nanoparticles on Conductive Carbon Support Boosts Oxidative Dehydrogenation of Hydroxymethylfurfural.....	110
<i>Bohyeon Kim, Mark Douthwaite, Issac T. Daniel, Liang Zhao, Xiaoyang Huang, Samuel Pattisson, Ouardia Akdim, Richard J. Lewis, Runjia Lin, Bingqing Yao, Kai Wang, Peter J. Miedziak, Greg M. Shaw, David J. Morgan, Sultan Althahban, Thomas E. Davies, Qian He, Christopher Kiely, Graham J. Hutchings, Steven McIntosh</i>	
687f Electrifying Hydroformylation Catalysts Exposes Voltage-Driven C–C Bond Formation	111
<i>Joy Zeng, Chenyu Jiang, Spencer Delgado, Jason S. Adams, Yuriy Román-Leshkov, Karthish Manthiram</i>	
687g Quantification of Catalytically Relevant Fe Species in Nitrogen-Doped Carbon	112
<i>Jason Bates, Jesse J. Martinez, Melissa N. Hall, Abdulhadi Al-Omari, Thatcher W. Root, Shannon S. Stahl</i>	

THERMAL AND THERMOCATALYTIC BIOMASS CONVERSION AND BIOREFINING I

703b Effects of Zeolite Framework on Direct Reduction of Ester to Ether Using H ₂ over Pt-Zeolite Catalysts	113
<i>Jieun Lee, Yang Sik Yun, Claudia Berdugo-Díaz, Jing Luo, David G. Barton, Xue (Ida) Chen, David Flaherty</i>	

703c Catalytic Strategy for Conversion of Triacetic Acid Lactone (TAL) to Potassium Sorbate.....	114
<i>Min Soo Kim, George Huber</i>	
703d Production of Neo Acids from Biomass-Derived Monomers.....	115
<i>Erha Andini, Jake Bragger, Sunitha Sadula, Dionisios Vlachos</i>	
703e Tuning the Selectivity of Aminosilica Catalysts for Aldol Reaction and Condensation to Produce Bio-Derived Surfactants	116
<i>Hannah Pineault, Nicholas Brunelli</i>	
703f Determining the Effect of Adsorbate-Adsorbate Intermolecular Interactions in the Adsorption and Decomposition of Binary Carboxylic Acid Mixtures on Pt(111).....	117
<i>Ayodeji Omoniyi, Samir Bensaid, Giuseppe Pipitone, Alyssa Hensley</i>	
703g Evaluation of Catalyst Deactivation Mechanisms during Direct Acylation of 2-Methylfuran with Acetic Acid over ZSM-5 Zeolites.....	119
<i>Ismaeel I. Alalq, Steven Crossley</i>	
703h Synergistic Catalysis of Metal Salt in Ionic Liquid on the Production of 5-Hydroxymethylfurfural from Glucose.....	120
<i>Yesub Keum, Huyen Tran Dang, Gunwoo Kim, Yong Jin Kim, Jayeon Baek</i>	

CATALYSIS AND REACTION ENGINEERING IN LIQUID AND MULTIPHASE SYSTEMS I: REACTION MECHANISMS

541a In-Situ Neutron Scattering of the Lignin Liquid-Phase Depolymerization with a Heterogeneous Catalyst.....	121
<i>Jialiang Zhang, Sai V. Pingali, Manju Mudiyansele, Marcus Foston</i>	
541b Solvation Effects on Carbonyl Group Hydrogenation over Transition Metal Catalysts.....	122
<i>Dia Sahseh, Paratee Komen, Andreas Heyden</i>	
541c Selective Hydrogenation of Alkyl-Substituted Phenols to Alkyl-Substituted Cyclohexanone over a Pd/Al ₂ O ₃ Catalyst Using a Three-Phase Flow Reactor	123
<i>Jimmy Soeherman, Paul J. Dauenhauer</i>	
541d Rational Tailoring of Solvent Recipes for Acid-Catalyzed Dehydration of Biomass-Derived Lactones	124
<i>Mohd Ussama, Gourav Shrivastav, Rachit Khare, Johannes A. Lercher, M. Ali Haider</i>	
541e Mapping the Coverage-Dependent Adsorption Energies of Complex Phenolics on Pd(111).....	125
<i>Naseeha Cardwell, Yong Wang, Jean-Sabin McEwen</i>	
541f Water-Assisted Hydrogenation of Aromatics Under Ambient Conditions over Ruthenium Catalyst: A Combined Experimental and Computational Investigation	127
<i>Bhanu Priya, Sagar Bathla, Ankit Kumar, Sanjay Singh, Samir H. Mushrif</i>	
541g Selective Reduction of O ₂ and H ₂ Via Hydroxyquinone Mediators in H ₂ O ₂ Synthesis.....	128
<i>Mayank Tanwar, Jason Adams, David Flaherty, Matthew Neurock</i>	

EMERGING CATALYTIC AND DYNAMIC REACTOR DESIGNS

672a 3D-Printed Capillary Force Trap Reactors (CFTRS) for Multiphase Catalysis Flow Chemistry	129
<i>Stella, Sze Yue Ng, David M. Walker, Joel Hawkins, Saif Khan</i>	

672b Quantifying Error Propagation in Microkinetic Predictions of Dynamic Rate Enhancement	130
<i>Sallye R. Gathmann, Paul J. Dauenhauer</i>	
672c Forced Dynamic Operation: Propene Ammoxidation over Bismuth Molybdate-Based Catalysts	131
<i>Zhuoran Gan, James Brazdil, Lars Grabow, William Epling</i>	
672d Kinetic Criteria for Non-Steady State Selectivity Enhancement during Ethane Oxidative Dehydrogenation	133
<i>Austin Morales, Michael Harold, Praveen Bollini</i>	
672e Catalytic Condensers for Programmable Catalysis.....	135
<i>Paul J. Dauenhauer</i>	
672f On the Dynamics of Electrification of Heterogeneous Catalytic Reactors	136
<i>Rucha Railkar, Kewei Yu, Weiqing Zheng, Dionisios Vlachos</i>	
672g Millisecond-Modulated Dynamic Gas Pulsing for Enhanced Surface Activity during Partial Oxidation of Methane to Syngas	137
<i>Fatou Baka Diop, Cameron Armstrong, Geoffrey Tompsett, Andrew R Teixeira</i>	
672h Investigating the Identifiability of Microkinetic Model Parameters with Transient Inputs	138
<i>Ran Wang, Zayne Weber, Robert Rioux, Michael Janik, Antonios Armaou</i>	

ELECTROCHEMICAL ENGINEERING: REACTOR DESIGN AND REACTION TRANSPORT PROCESSES IN ELECTROCATALYSIS I

670a A Novel Circuit-Based Model of a Bipolar Membrane Electrodialysis Reactor for Offshore Chemical Synthesis	139
<i>Jack Ledingham, Kyra Sedransk Campbell, Alasdair Campbell</i>	
670b A Two-Dimensional Transport Model of Bipolar Membrane Electrodialysis for the Electro-Regeneration of Carbon Capture Solvents.	140
<i>Jack Ledingham, Kyra Sedransk Campbell, Alasdair Campbell</i>	
670c A Systematic Analysis of the Electrochemical Reduction of CO ₂ Using Uncertainty Quantification.....	141
<i>Hariharan R K, Vedha Vaishnavi R, Himanshu Goyal</i>	
670d Coupling Microkinetics with Continuum Transport Models to Understand Electrochemical CO ₂ Reduction	142
<i>Nitish Govindarajan, Joel B. Varley, Tiras Lin, Thomas Roy</i>	
670e Bipolar Membrane Electrolyzers Architectures for Ion Transport Control and Impure Water Electrolysis	143
<i>Adam Nielander, Daniela Marin, Joseph Perryman, Thomas F. Jaramillo</i>	
670f Understanding the Effects of Microenvironment and Mass Transport on Electrochemical CO ₂ Reduction Using Operando ATR-Seiras	144
<i>Jesse Matthews, Jaime Aviles Acosta, Adam Nielander, Thomas F. Jaramillo</i>	
670g Development of Reaction-Transport Kinetics Model for Electrochemical CO ₂ Reduction on Copper: Moving Away from Tafel Kinetics to Incorporate Mass Transfer Effects.....	145
<i>Joonbaek Jang, Carlos Morales-Guio</i>	

670h Resolving Local Microenvironments and Fluxes in Electrochemical CO ₂ Reduction Using Continuum Modeling.....	146
<i>Justin Bui, Alex J. King, Adam Weber, Alexis T. Bell</i>	

CATALYTIC UPCYCLING OF WASTE PLASTICS I: PYROLYSIS AND GASIFICATION

633a Upcycling Plastic and Coal Wastes into Syngas By Steam Gasification	147
<i>Sittichai Natesakhawat, Nicholas C. Means, Victor Abdelsayed, Jennifer Weidman, Fan Shi, Jonathan Lekse, McMahan L. Gray, Ping Wang</i>	
633b Oxidative Cleavage of Waste Polyolefins As a Route to Recycled-Carbon Polar Waxes.....	148
<i>Hyunjin Moon, Fumihiko Shimizu, Kazuki Fukumoto, Hengbin Wang, Xiangcheng Sun, Susannah L. Scott</i>	
633c Molecular Recycling: Catalytic Pyrolysis of Plastic Waste	149
<i>Kevin Van Geem</i>	
633d Radical Initiated Thermal Depolymerization of Polystyrene.....	150
<i>Elizabeth Belden, Alex Maag, Michael T. Timko</i>	
633e Assessing the Kinetics of Solid Waste Pyrolysis Under Catalytic and Non-Catalytic Conditions Using Thermogravimetric Analysis.	151
<i>Naif Raja, Gloria Milena Monsalve-Bravo, Muxina Konarova</i>	
633f Exploring the Potential of Co-Upcycling PS and PE for Enhanced Aromatics Production	152
<i>Thang Luong, Yuxin Wang, Jianli Hu</i>	
633g Catalytic Upcycling of Oxygenated Polymers with MFI Type Zeolites	153
<i>Kanan Shikhaliyev, Thossaporn Onsree, Jochen Lauterbach</i>	
633h Determining the Effect of Pyrolysis Operating Conditions on the Catalytic Co-Pyrolysis of Ldpe and PET with Zeolite Catalysts	154
<i>Sean Okonsky, Neil Hogan, Hilal Ezgi Toraman</i>	

CO₂ UPGRADING I: MECHANISTIC INSIGHT

646a Directing the Selectivity of CO ₂ Electroreduction Toward a Single C ₂ Product By Collective Control of Rate-Determining and Selectivity-Determining Steps	155
<i>Jingjie Wu</i>	
646b Tuning Amine-Based Polymer Catalyst for CO ₂ Conversion through Structural Modification Via Quaternization.....	156
<i>Alejandro Chaperro-Planell, Hui Xu, Renxi Jin, Casey O'Brien</i>	
646c Co-Adsorbed Surface Hydroxide and CO Promote CO ₂ Electrolysis to Ethylene in Acidic Conditions	157
<i>Zhu Chen, Yufei Cao, David Sinton, Jun Ge, Edward Sargent</i>	
646d Rates and Reversibility for CO ₂ Hydrogenation on Cu-Based Catalysts	158
<i>Ting Lin, Aditya Bhan</i>	
646e Computational Investigation into Supported and Inverted Cu-ZrO ₂ Catalysts for Selective Conversion of CO ₂ to Methanol	159
<i>Anshuman Goswami, Junjie Chen, Alessandro Gallo, Thomas F. Jaramillo, Frank Abild-Pedersen</i>	

646f Understanding Hydrogenation of CO/CO ₂ Mixtures to Light Hydrocarbons over Ru-Co Single Atom Alloys Via Low-Temperature Fischer Synthesis.....	160
<i>John El Berch, Renjie Liu, Stephen House, Samuel Meil, Marc Porosoff, Giannis Mpourmpakis</i>	
646g Commodifying Flue Gas: Molten-Carbonate-Assisted Olefin Synthesis	161
<i>Kyle Vogt-Lowell, Kunran Yang, Dennis Chacko, Arnab Bose, Jace Carsten, Junchen Liu, Matthew Housley, Fanxing Li</i>	
646i Solvation Effects for Nonaqueous CO ₂ Electrochemistry	163
<i>Chibueze Amanchukwu</i>	

DATA SCIENCE AND MACHINE LEARNING APPROACHES TO CATALYSIS I: DATA-ENHANCED MULTISCALE SIMULATIONS

661a Data Science and Machine Learning Approaches to Catalysis	164
<i>John Kitchin</i>	
661b Competition between Mononuclear and Binuclear Copper Sites across Different Zeolite Topologies	165
<i>Asanka Wijerathne, Allison Sawyer, Rohil Daya, Christopher Paolucci</i>	
661c Developing Physically Meaningful and Accurate Machine Learning Interatomic Potentials for Catalysis	166
<i>Tristan Maxson, Ademola Soyemi, Tibor Szilvasi</i>	
661d Using Neural Networks to Interpret Transient Kinetic Data.....	167
<i>Andrew Medford, Gabriel Gusmão, Dingqi Nai</i>	
661e Modeling Supported Sub-Nanometer Cluster Catalysts Via Multiscale Computations and Machine Learning.....	168
<i>Salman A. Khan, Stavros Caratzoulas, Dionisios Vlachos</i>	
661f Towards Domain-Informed Machine Learned Models from High Throughput Experimental Data	169
<i>Klea Ziu, Martin Takac, Srinivas Rangarajan</i>	

ELECTROCATALYSIS AND PHOTOCATALYSIS III: ELECTROCATALYTIC TRANSFORMATION OF ORGANIC MOLECULES

666a Oxidation By Reduction: Electrocatalytic Reduction of Peroxydisulfate for Efficient and Selective Oxidation of Alcohols	170
<i>Mayank Tanwar, Seyyedamirhossein Hosseini, Jordyn Janusz, Andrew Pendergast, Henry White, Matthew Neurock</i>	
666b Elucidating the Mechanism of Electrocatalytic Alkane Fragmentation and Oxidation Using Time-Dependent Potential Profiles.....	171
<i>Christine Lucky, Marcel Schreier</i>	
666c Rate Enhanced and Energy-Efficient Electrocatalytic Oxidation of Formic Acid: A Dynamic Duo for Sustainable Catalysis.....	172
<i>Faviola Villariny-Rosado, Omar Abdelrahman</i>	

666d Reaction Mechanism of Electrochemical Alkene Epoxidations in Aqueous-Organic Electrolyte	173
<i>Richa Ghosh, Drew Hollyfield, David Potts, Raghuram Gaddam, Joaquín Rodríguez-López, David Flaherty</i>	
666e Direct Propylene Epoxidation Via Water Activation over Electrocatalysts	174
<i>Minju Chung, Joseph Maalouf, Jason S. Adams, Yuriy Román-Leshkov, Karthish Manthiram</i>	
666f Electrochemical Synthesis of Aniline Using Ammonia and Benzene	175
<i>Ishita Goyal, Meenesh R Singh</i>	
666g Simulating Chemical Reactions at Working Electrode Interfaces with Constant Potential Neural Network Potentials	176
<i>Amro Dodin, Phillip Geissler, David Limmer</i>	

ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS I: EMERGING CATALYTIC TECHNOLOGIES

673a SO ₂ Interactions with Hydrothermally Treated Colloidal Pd-Based Catalysts: Influence of Particle Size on SO ₂ Poisoning.....	177
<i>Natalia Diaz Montenegro, Grayson Johnson, Zhuoran Gan, William Epling</i>	
673b Silver Single Atom Catalysts on Different Supports with Distinct Catalytic Performance for the Selective Oxidation of Ammonia.....	178
<i>Kailong Ye, Shaohua Xie, Tyler Campbell, Duy Le, Talat S. Rahman, Fudong Liu</i>	
673c Elucidating Redox Pathways for Nitrous Oxide Emissions Control over Metal-Zeolite Catalysts	180
<i>Siddarth Krishna, Libby Brungardt, Vaishnav Sunkireddy</i>	
673d Reaction and Structural Dynamics in Aqueous Pollutant Degradation By Earth-Abundant Metal-Organic Frameworks.....	181
<i>Samuel C. Moore, Michele Sarazen</i>	
673e Dynamic Modulation of Surface Carbon and Oxygen Vacancies for Sustained Chemical Looping Production of Syngas on 5wt.%Ni/Ce _{0.6} Zr _{0.4} O ₂ Catalyst	182
<i>Debtanu Maiti, Zoe C. Benedict, M. Ross Kunz, Sherafghan Iftikhar, Yixiao Wang, Fanxing Li, Yingchao Yang, Rebecca Fushimi</i>	
673f Novel Design of Cobalt Oxide Catalyst Supported on γ -Alumina Using Simple Dehydroxylation Method.....	183
<i>Sang Woo Byun, Hyeonwoo Shin, Jiseok Park, Sung Bong Kang</i>	
673g Aqueous Formiate-Bicarbonate for Hydrogen Storage.....	184
<i>Danilo Russo, Marcella Calabrese, Roberto Andreozzi, Almerinda Di Benedetto, Raffaele Marotta</i>	
673h Water Induced Ammonia Production on CuO/Al ₂ O ₃ Catalyst in NO + CO Reaction	186
<i>Wei Tan, Shaohua Xie, Lin Dong, Fudong Liu</i>	

FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE I: CATALYSIS OVER OXIDES AND NITRIDES

675a Rate Analysis Implications of (Side) Product Inhibition in Mars-Van Krevelen Redox Cycles	188
<i>Xiaohui Zhao, Jeffrey Rimer, Praveen Bollini</i>	

675b Oxidative Dehydrogenation of Ethane over Boron Containing Chabazite	190
<i>Mi Jen Kuo, Raul Lobo</i>	
675c Heterogenous Propylene Metathesis over Molybdenum Silicate Microspheres with Dispersed MoO _x Sites	191
<i>Ran Zhu, David Škoda, Barbora Hanulíková, Ales Styskalik, Vít Vykoukal, Petr Machač, Lucie Simonikova, Ivo Kuřitka, Claude Poleunis, Damien P. Debecker, Yuriy Román-Leshkov</i>	
675d Insights into the Structure-Activity Relationship of Cu-Doped Ceria for Reverse Water-Gas Shift Reaction: A Combined Theoretical and Experimental Investigation	192
<i>Shang Jiang, Kishore Kandasamy, David Simakov, Samir H. Mushrif</i>	
521ao Strain-Dependent Activity and Stability of RuO ₂ and IrO ₂ Oxygen Evolution Catalysts	193
<i>Payal Chaudhary, Alexandra Zagalskaya, Vitaly Alexandrov</i>	
675f Convex Hulls in Computational Catalysis	194
<i>Gregory Collinge</i>	
675g Descriptors for Rates and Selectivities of H ₂ and C _x H _y Combustion on Bi ₂ O ₃	196
<i>Matthew Jacob, Aditya Bhan</i>	
675h Determining Promoter Effects in the Nanoscale Surface Structure and Stability of NiO-Based Catalysts for Ethane Oxidative Dehydrogenation	197
<i>Shuqiao Wang, Alyssa Hensley</i>	

HYDROCARBON CONVERSION I: INSIGHTS FROM MODELING AND THEORY

681a A Combined Experimental and Theoretical Investigation of CO ₂ Assisted Alkane Oxidative Dehydrogenation over Ceria-Based Catalysts	198
<i>Gouri Ramadas Nayanar, Anoop P Pushkar, Jithin John Varghese, Niket Kaisare</i>	
681c Insights of Structure-Property Relationships of Pt-Sn and Pt-Zn Bimetallic Catalysts for Propane Dehydrogenation	199
<i>Yilang Liu, Xue Zong, Stavros Caratzoulas, Dionisios Vlachos</i>	
681d Controlling the Activation of Methane for the Value-Added Products on Ir-Doped RuO ₂ and TiO ₂ (110).....	200
<i>Jisu Shin, Omar Almarshad, Christopher Lee, Suriya Ramasubramian, Jason F. Weaver, David Hibbitts</i>	
681e Tuning Single Atom Catalyst - Support Interactions for Facile Methane Activation.....	202
<i>Paige Shumskas, Hilal Ezgi Toraman, Michael Janik, Konstantinos Alexopoulos</i>	
681f Mechanistic Studies of Roles of Extra-Framework Species in MFI Zeolite on Catalytic Cracking of Propane	203
<i>Jacob Crouch, Bin Wang</i>	
681g Carbon-Based Catalysts for Non-Oxidative Coupling of Methane	204
<i>Luke Pretzie, Jeffrey Greeley</i>	
681h The Influence of Sulfur Promoters on the Morphology and Reactivity of Pt Nanoparticles for Methyl Cyclohexane Dehydrogenation	205
<i>Asmee Prabhu, Chuhong Lin, Uzma Anjum, Xin Zhao, Voon Huey Lim, Rong Xu, Tej Choksi</i>	

COMBUSTION KINETICS AND EMISSIONS

659a Nitrogen Oxide Mitigation Via a Waste-derived Heterogeneous Mixed Metal Oxide.....	207
<i>Kaitlyn Lawrence, Marco J. Castaldi</i>	
659b Development and Application of Detailed Kinetics Mechanisms for PFAS Incineration	208
<i>Phillip Westmoreland, Hrishikesh Ram, Thomas P. Sadej, C. Claire Murphy, Tim J. Mallo</i>	
659d Exploring Combustion Chemistry of 4-Methyl-1-Pentene in Pyrolysis and Laminar Flame Propagation with into Fuel Isomeric Effects of C ₆ Alkenes	210
<i>Chuangchuang Cao, Qilong Fang, Wang Li, Jianguo Zhang, Wei Li, Long Zhao, Jiuzhong Yang, Yuyang Li</i>	
659f Reducing Nitrous Oxide Emissions in the Ostwald Process Via a Combined Experimental and Statistical Approach.....	211
<i>Lars-Christian Stoltenberg, Felix Kornemann, Felix Biermann, Artur Wiser, Christian Renk, Andreas Orth, Alfons Drochner, Martin Votsmeier, Bastian Etzold</i>	
659h Modifying the Electronic Environment of VO _x Active Site By Altering the Support Structure to Improve Hg Oxidation Activity.....	213
<i>Woonsuk Yeo, Dongjae Shin, Jeong Woo Han</i>	

GREEN CHEMICAL REACTION ENGINEERING FOR SUSTAINABILITY

680a Ecofriendly Biolubricant Production from Waste Cooking Oil and Lignocellulosic Biomass- Derived Oxygenates	214
<i>Hossein Jahromi, Sushil Adhikari</i>	
680b Intensification of Renewable 4,4'-Dimethylbiphenyl Synthesis Via Oxidative Coupling and Tandem Diels-Alder and Dehydration of 2-Methylfuran	215
<i>Charles Fields IV, Mi Jen Kuo, Yuqing Luo, Raul Lobo, Dionisios Vlachos</i>	
680c Kinetic Modelling and Measurement of Catalyst Deactivation for the Catalytic Co-Pyrolysis of PP and PET with HZSM-5	216
<i>Sean Okonsky, J.V. Jayarama Krishna, Hilal Ezgi Toraman</i>	
680d Efficient Degradation of Perfluoroalkyl Acids in Phytoremediation Wetlands: A Novel Catalytic Hydrothermal Liquefaction Approach.....	217
<i>Wenjia Wang, Hongbiao Du</i>	
680g Understanding and Improving the Synthesis of Starbon® Materials from Low Amylose Content Starches for Its Use As Catalyst.....	218
<i>Milena Zabala, Alvaro Orjuela, Alexandra Inayat, Katrin Städtke, Laura Panqueba</i>	
680f The Effects of Solvent Properties on Radical Formation from Ultrasound-Driven Inertial Cavitation for Sono-Chemical Process Intensification.....	219
<i>Ari Fischer, Robert Maligon Querimit, Tej Choksi</i>	

MODELING AND ANALYSIS OF CHEMICAL REACTORS

692a Forced Dynamic Operation for Enhanced Conversion during Methane Oxidation on Dual- Layer Pt/Pd + Mn _{0.5} Fe _{2.5} O ₄ Spinel: Kinetic and Reactor Modeling	221
<i>Pak Wing Chen, Lars Grabow, Michael Harold</i>	

692b Shallow-Bed Reactor Design and Analysis for the Autothermal Oxidative Dehydrogenation of Ethane over Mordenite Catalysts.....	222
<i>Jiakang Chen, Praveen Bollini, Vemuri Balakotaiah</i>	
692c Multistability in Membrane Reformers Due to Permeance Inhibition By Competitive Adsorption of CO	223
<i>Maria Anna Murmura, Antonio Brasiello</i>	
692d Using Magnetic Resonance Imaging (MRI) As a Full-Field Validation Technique for Reactive CFD Simulations.....	224
<i>Kevin Kuhlmann, Harm Ridder, Ingmar Bösing, Georg R. Pesch, Jorg Thöming</i>	
692e Kinetic Model Building through Simultaneous Optimization from Spectral Data	225
<i>Thomas Krumpolc, Daniel W. Trahan, Xiaoyun (Shawn) Chen, Lorenz T. Biegler</i>	
692g Evaluating Hydrodynamic and Homogeneous Buffer Reaction Effects on the Electrochemical Hydrogen Evolution Reaction Using Experimentally Validated CFD Simulations.....	226
<i>Derek Richard, Matthew Tom, Sungil Yun, Joonbaek Jang, Panagiotis Christofides, Carlos Morales-Guio</i>	

MULTI-SCALE MODELING

693b Analyzing the Uncertainty of Linear Scaling, Machine Learning, and DFT Derived Thermodynamics for the Catalytic Partial Oxidation of Methane on Rhodium 111.....	227
<i>Chao Xu, Christopher Blais, Richard West</i>	
693c Elucidating the Nanoscale Driving Forces for Environment-Driven Rh-Pd Nanoparticle Reconstruction.....	228
<i>Shuqiao Wang, Alyssa Hensley</i>	
693d Polymer Upcycling By Tandem End-Scission and Random Scission Catalysts: Model and Analysis of Experiments.....	229
<i>Ziqiu Chen, Baron Peters</i>	
693e Multi-Scale Simulation of Non-Catalytic Gas-Solid Reactions in Counter-Current Moving-Bed Reactors.....	230
<i>Patricia Metolina, Anthony Dixon, Roberto Guardani</i>	
693f Stability and Reactivity of Encapsulated Monomeric and Dimeric Pt Clusters in Chabazite Framework.....	232
<i>Sanjana Srinivas, Stavros Caratzoulas, Dionisios Vlachos</i>	
693g Impact of Particle Shape and Orientation on the Intraparticle Physicochemical Phenomena of Catalytic Particles.....	233
<i>Stylianos Kyrimis, Robert Raja, Lindsay-Marie Armstrong</i>	
693h Effect of Scale-up on Mass Transfer and Flow Patterns in Liquid-Liquid Microchannels Using Experiments and Computations.....	235
<i>Arnav Mittal, Matthew Marino, Souryadeep Bhattacharyya, Tai-Ying Chen, Pierre Desir, Dionisios Vlachos, Marianthi Ierapetritou</i>	

REACTION CHEMISTRY AND ENGINEERING I

699a Scalable Photoreactors Using Intensified Wireless Micro LED Packed Beds	236
<i>Esai Lopez, Andrew R Teixeira</i>	

699b Exploration of Novel Catalysts for Dehydrogenation of Methylcyclohexane.....	237
<i>Thossaporn Onsree, Kaveh Shariati, Kenneth Roberts, Jochen Lauterbach, Azadeh Mehrani</i>	
699c Continuous-Flow Microfluidic Device to Screen CO ₂ Capture Efficiency of Carbonation of Industrial Mineral Waste.....	238
<i>Vamsi Vikram Gande, Meenesh R Singh</i>	
699d One-Pot Mechanochemical Hydrogenation and Acetylation of 4-Nitrophenol to Paracetamol with a Multi-Phase Ball Mill Reactor.....	240
<i>Jimin Park, Jacob Maier, Marta Hatzell, Carsten Sievers, Andy Bommarius</i>	
699e At-Line Monitoring of Diphenhydramine Synthesis Via Low-Field NMR Spectroscopy As Process Analytical Technology.....	241
<i>Jakub Konkol, Ravendra Singh, Fernando Muzzio, George Tsilomelekis</i>	
699f Engineering Strategies to Control Liquid Phase Oxidation of Hydrocarbons to Produce Value-Added Chemicals	243
<i>Muhammad Siddiquee</i>	
699g Reduction of a Detailed Kinetic Mechanism of the Pyrolysis of Acetylene.....	247
<i>Fatima Matamoros, Roda Bounaceur, Hubert Monnier, Pierre-Alexandre Glaude, Abderrazak Latifi</i>	

REACTION ENGINEERING IN PHARMACEUTICALS AND FINE CHEMICALS

701a Development of a Chiral Catalyst Immobilized Continuous Flow Process for a Key Asymmetric Hydrogenation Step of an API Synthesis.....	249
<i>Aibolat Koishybay, Ahmet Aloglu, Xinlei Huang, Keith Barbato, Hannah Nguyen, Chuntian Hu, Stephen Born</i>	
701c Process Elucidation and Hazard Analysis of Metal-Organic Framework Scale-up Synthesis: A Case Study of ZIF-8	250
<i>Yufeng Quan, Qingsheng Wang</i>	
701d Innovative Applications for Effective Biocatalysis in Continuous Flow.....	251
<i>Alessia Valotta, Heidrun Gruber-Woelfler</i>	
701e An Autonomous Microreactor Platform for the Rapid Identification of Kinetic Models for Fast Liquid/Liquid Reactions	253
<i>Anna Katsarou, Arun Pankajakshan, Jonathan Lefebvre, Julia Hofinger, Federico Galvanin, Alexei A. Lapkin</i>	
701f Process Development of a Piperidine Fragment for a Pipeline Asset: A Story Centered at the Interface of Carboxylation and Hydrogenation Chemistries	254
<i>Jeremy Griffin, Simon Velasquez Morales, Greg Storer, Ryan Ellis, Wakuna Galega, Jeremy Henle, Steve Richter, Kaid Harper</i>	
701h Pharmaceutical Synthesis in Flow – Process Intensification of Albuterol.....	255
<i>Daniel Gregory, Kaitlin Kay, Justin Turnage, Brandyn Kimball, Jeffrey Noble, Frank Gupton, James K. Ferri</i>	
Controllable Photocatalytic Molecular Oxygen Oxidation Based on Sulfur-Containing Photosensitizers	256
<i>Jingnan Zhao, Qingwei Meng</i>	

REACTION PATH ANALYSIS

702a Recent Advances in Predictive Kinetics	257
<i>William Green, Xiaorui Dong, Hao-Wei Pang, Yen-Ting Wang, Kevin Spiekermann, Haoyang Wu, Yunsie Chung, Angiras Menon</i>	
702b Discovery of Novel Pathways Using Artificial Intelligence	258
<i>Quan Zhang, William W. Sprague, Linda Broadbelt</i>	
702c Microkinetic Elucidation of the Ethylene Hydroformylation Mechanism on a Heterogenized Rh-Based MOF Catalyst.....	259
<i>Sébastien Siradze, Jeroen Poissonnier, Silje F. Håkonsen, Morten Frøseth, Richard H. Heyn, Joris W. Thybaut</i>	
702d Intramolecular Catalytic Hydrogen Atom Transfer (CHAT): A Novel Mechanism Relevant to the Combustion of Traditional Fuels	261
<i>Rubik Asatryan, Venus Amiri, Jason Hudzik, Mark Swihart</i>	
702e Explaining Gas Evolution Mechanisms in Mg-Ion Batteries with Chemical Reaction Networks	262
<i>Evan Spotte-Smith, Samuel M. Blau, Daniel Barter, Noel Leon, Nathan Hahn, Nikita Redkar, Kevin Zavadil, Chen Liao, Kristin Persson</i>	
702f Investigation of Liquid Fuel Generation from Carbon Dioxide over Bimetallic Systems	263
<i>Yuting Xu, Michael Ross, Fanglin Che</i>	
702g Investigation on the Role of Acidity for NH ₃ Selective Catalytic Reduction of NO on Mo/Fe ₂ O ₃ single Atom Catalyst.....	264
<i>Tamilmani Selvaraj, Preeti Aghalayam, Jithin John Varghese</i>	

INTENSIFIED PROCESSES II

685a Design and Analysis of Electrically Heated Reactors for Endothermic Chemistries.....	265
<i>Vemuri Balakotaiah</i>	
685b Scalable, Volumetric Electrified Heating with High Frequency Magnetic Induction.....	266
<i>Jonathan Fan, Calvin Lin, Dolly Mantle, Zhennan Ru, Pinak Mohapatra, Ariana Hofelmann, Chenghao Wan</i>	
685c Codesign of Multijunction Photoelectrochemical Devices for Unassisted CO ₂ Reduction to Multicarbon Products	267
<i>Alex King, Adam Weber, Alexis T. Bell</i>	
685e Techno-Economic Optimization of a Microwave-Assisted Methane Dehydroaromatization Process.....	268
<i>Harish Damahe, Md Emdadul Haque, Debangsu Bhattacharyya, Jianli Hu</i>	
685f Deciphering the Roots of Catalyst Degradation in Electrochemical CO ₂ Reduction Via Interpretable AI.....	269
<i>Daeun Shin, Hakan Karasu, Dahye Won, Jonggeol Na, Ung Lee</i>	
685g Numerical Modeling of Microwave-Assisted Catalytic Conversion of Natural Gas: The Role of SiC and Coke Deposition on Microwave Absorption	270
<i>Xinwei Bai, Pranjali Muley, Victor Abdel-Sayed, Daniel Haynes</i>	

INTENSIFIED PROCESSES I

684c Optimization and Screening of Iron-Supported on Clinoptilolite As a Low-Temperature Fischer-Tropsch Synthesis Catalyst.....	271
<i>Roick Chikati, Joshua Gorimbo, Diakanua Nkazi</i>	
684d Autonomous Homogeneous Catalysis Enabled By a Self-Driving Flow Reactor	272
<i>Jeffrey Bennett, Milad Abolhasani</i>	
684e Hydrothermal Liquefaction of Wet Organic Wastes Using Sub-Stoichiometric Homogenous Oxidant	273
<i>David Kenney, Timothy Woodard, Julian Bennett, Andrew Charlebois, Aidin Panahi, Andrew R Teixeira, Michael T. Timko</i>	
684f Temperature-Dependent Global Kinetic Rate Parameters for the Production of Polycyclic Aromatic Hydrocarbons from the Supercritical Pyrolysis of Ethylcyclohexane	274
<i>Avinash Mali, Mary J. Wornat</i>	
684g An Experimental Investigation of Parallel Free-Radical and Ionic Reaction Kinetics of Propane Oxidation in Supercritical Water	275
<i>Andrew Mansfield, Nanta Sophonrat</i>	

POSTER SESSION: CATALYSIS AND REACTION ENGINEERING (CRE) DIVISION

Outer Solvation Shell Towards Zn Ion Battery.....	276
<i>Qianyi Ma</i>	
521a Continuous 5-HMF Production in a Biphasic System Using Mesoporous Aluminosilicate Functionalized with Acid.....	277
<i>Gunwoo Kim, Hye Jin Lee, Yesub Keum, Yong Jin Kim, Jayeon Baek</i>	
521b Red Mud As a Catalyst and Oxygen Carrier in Biomass Gasification: A Route to Recover Iron from Bauxite Residue	278
<i>Pedro Souza, Nardana Bazybek, Efthymios Kantarelis, Frederico Penha, Klas Engvall, Shareq Mohd Nazir</i>	
521c Transition-Metal-Phosphide-Decorated De-Aluminated Zeolites As Regenerable and Deactivation-Resistant Biomass Pyrolysis Catalysts.....	279
<i>David Ojo, Theodore Walker</i>	
521e Biochar Catalyst Screening for Enhancing Energy Recovery from Pyrolysis	280
<i>Zhongzhe Liu</i>	
521f Investigating the Effect of Micropore Content on Catalytic Activity and Selectivity for Glucose Isomerization to Fructose	281
<i>Paul Neff, Nitish Deshpande, Hannah Pineault, Jee-Yee Chen, Nicholas Brunelli</i>	
521g Selective Hydrogenation of Phenol in Aqueous Phase over Organically Modified Silica Support: Effect of Basic Site Incorporation.....	282
<i>Snehal Patil, Anagha Hunoor, Paul Edmiston, Umit Ozkan</i>	
521h Stability of Zeolite Y in Aqueous Media: Framework Degradation Under Ambient Temperature and Pressure.....	283
<i>Anya Zornes, Omio Das, Jeffery White</i>	

521i Optimization of Process Parameters for Solketal Synthesis Using Microwave Reactor: Catalytic Activity and Reactor Energy Model.....	284
<i>Mousumi Chakraborty, Arun Kumar Jana, Megha Vichare</i>	
680e 12-Tricosanone Production from Lauric Acid for the Synthesis of Cellulosic Base Oils	286
<i>Tejas Goculdas, Zhifei Yuliu, Sunitha Sadula, Weiqing Zheng, Arvind Nanduri, Basudeb Saha, Marianthi Ierapetritou, Dionisios Vlachos</i>	
521j Reaction Regimes in Interfacial Polyamidation and Their Effect on Film Properties	287
<i>Akkihebbal K. Suresh, Preeti Jha</i>	
521eu Catalytic Upcycling of Polyolefin Wastes Using W-Based Polyoxometalates	289
<i>Hongda Zhu, Bala Subramaniam</i>	
521k Non-Enzymatic, Resonance-Promoted Bio-Renewable Polymer Production Under Mild Conditions.	290
<i>Shayan Hosseini, Theodore Walker</i>	
521m Molecular Design of Polymer-Modified Catalyst Supports for Improved Bio-Renewable Energy Processes: Theory, Synthesis and Experiments.....	291
<i>David Moses, Theodore Walker</i>	
521n Selective Reduction of Alkyl-Substituted Phenols to Alkyl-Substituted Cyclohexanone over a Pd/Al ₂ O ₃ Catalyst Using a Three-Phase Flow Reactor.....	292
<i>Jimmy Soeherman, Paul J. Dauenhauer</i>	
521o Understanding the Adsorptive Behavior of Polymeric Materials to Catalyst Surfaces Using Various X-Ray Methods	293
<i>Erin Dunphy, Michael F. Toney, J. Will Medlin, Ziyue Dong, Kayla Sprenger</i>	
521p Mechanistic Understanding of the Efficient Hydrocracking of Waste Polyethylene on Two-Dimensional Pt/WO ₃	295
<i>Qimin Zhou, Deliang Wang, Qingyue Wang, Pingwei Liu</i>	
521q Computer Aided Molecular Design Coupled to Deep Learning Techniques As a Less-Expensive Approach to Design Organic Photoredox Catalysts	296
<i>Antonio Flores-Tlacuahuac, Alan Aguirre-Soto</i>	
521s Structure - Activity Relationship of Ni-Ru/ γ -Al ₂ O ₃ Catalyst for CO ₂ Methanation Reaction.	298
<i>Sairam S, Yacham Ashok, Jithin John Varghese, Tarak Patra, Preeti Aghalayam</i>	
521t Tuning Product Selectivity of Electrochemical CO ₂ Reduction in Acid Electrolyte Using Cu Nanoparticles on Surfactant-Treated Carbon.....	299
<i>Hwiyeon Noh, Yoonsun Park, Brian M. Tackett</i>	
521w Characterization of CO ₂ Binding and Reaction Mechanisms on Alkaline Dual Function Materials (DFMs) for Reactive Carbon Capture to Useful C1 Products	300
<i>Chae Jeong-Potter, Daniel Ruddy</i>	
521x Density Functional Theory Study for Ethylene Production from CO ₂ on Cu/TiO ₂ Photocatalyst	301
<i>Hayoung Jeong, Jeong Woo Han</i>	
521z CO ₂ cycloaddition with Epoxide into Cyclic Carbonates Using Zeolitic Imidazolite Frameworks: Effects of Defect Centres, Surface Sites and Ionic Liquids	302
<i>Athira Kelothum Kandi, Jithin John Varghese, Parasuraman Selvam</i>	

521aa Towards Controlling the Morphology of Nanostructured Carbons Via CO ₂ Electroreduction in Molten Salt Electrolyte.....	303
<i>Andrew Wong, Fei Yu</i>	
521ab Investigating Corrosion Dynamics during CO ₂ Reduction Using Inductively-Coupled Plasma Mass Spectrometry.....	304
<i>Katherine Yan, Kyra Yap, Gaurav A. Kamat, Michaela Burke Stevens, Adam Nielander, Thomas F. Jaramillo</i>	
521ac Molecular Catalyst-Functionalized Silicon Photocathode for Aqueous Photoelectrocatalytic CO ₂ Reduction to Methanol	305
<i>Bo Shang, Hailiang Wang</i>	
521ae Development of High-Efficiency Catalysts for Light Olefin Production through CO ₂ Hydrogenation over Fe-Based Catalysts	306
<i>Haewon Jung, Hermawan Prajitno, Jeongtak Kim, Soon Kwan Jeong, Ki Bong Lee, Sun-A Choi, Sun-mi Hwang</i>	
521af Tuning Oxygen Vacancies in Ni/CeO ₂ for CO ₂ Methanation	307
<i>Miguel Sepulveda, Elspeth Petersen, Yomaira Pagan Torres</i>	
655g Magnetically Enhanced Electrochemical Reduction of CO ₂ to Syngas.....	308
<i>Cristina González-Fernández, Nathan W. Wilson, Eugenio Bringas, Inmaculada Ortiz, Gerardine G. Botte, Jenifer Gomez Pastora</i>	
521ah Electrode Design Parameters Optimization of NCM622 Cathode in Lithium-Ion Battery for High Energythe Electrode Design	309
<i>Mohammed Atwair, Ali Cherif, Chul-Jin Lee</i>	
521aj Thermodynamic and Electronic Properties of MoSi ₂ N ₄ Edges	310
<i>Atharva Barte, Ashwin Ramasubramaniam, Omar Abdelrahman</i>	
521ak Impact of Electrolytes on the Adsorption of Phenol on a Platinum Electrode.....	312
<i>Ankit Mathanker, Wendy Yu, Isaiah Barth, Nirala Singh, Bryan Goldsmith</i>	
521am Selective Water Oxidation to H ₂ O ₂ on Mn-Alloyed TiO ₂ Surfaces	313
<i>Devan Solanki, Ke Yang, Victor S. Batista, Shu Hu</i>	
521an High Throughput Workflow for Electrocatalysis in Single Atom 2D Materials	315
<i>Richard Tran, Najmeh Honari, Lars Grabow</i>	
521ap In-Situ Analysis of Electrocatalytic Conversion of 5-Hydroxymethylfurfural (HMF) By Scanning Electrochemical Microscopy (SECM).....	316
<i>Seokjun Han, Won Tae Choi</i>	
521aq Bifunctional Fe/Co 2D Metal Organic Framework for Enhanced ORR and Oer Activity.....	317
<i>Naomi Helsel, Pabitra Choudhury</i>	
521as Carbon Quantum Dots for Sustainable Energy Conversion: Investigating Electrocatalytic and Photoelectrochemical Properties of Carbon Quantum Dots	318
<i>Zhikui Wang, Won Tae Choi</i>	
521at Controllable Photocatalytic Molecular Oxygen Oxidation Based on Sulfur-Containing Photosensitizers in Continuous Flow	319
<i>Jingnan Zhao, Qingwei Meng</i>	

521au Excellent Anion Exchange Membrane Electrolyser with Highly Active Oxygen Evolution Reaction Nife-LDH Self-Support Electrode.....	320
<i>Yingjie Feng, Xiaoyue Fu, Yuxiu He, Yue Zhou, Junfeng Zhang, Yan Wang, Qingrui Zhao, Jing Feng, Dongbing Liu, Jie Bai, Fan Li</i>	
521aw Electrochemically Assisted Activation of Light Alkanes at Ambient Conditions	321
<i>Wenxuan Liu, Qi Lu</i>	
521ax Reaction Pathways for the Electrochemical Oxidation of Cyclohexane to KA Oil	322
<i>Tana Siboonruang, Maureen Tang</i>	
521ay Understanding the Acid Electrolyte Anion Adsorption Effects for Oxygen Electrocatalysis	323
<i>S. A. Keishana Navodye, G. T. Kasun Kalhara Gunasooriya</i>	
521az Local pH Change during Alkaline HER Electrolysis with Electrodeposited Co-Mo-Based Titania Composite Electrocatalysts	324
<i>Elizabeth Podlaha-Murphy, Cheng Wang</i>	
521ba High-Resolution Kinetic Analysis of Photocatalytic Water Splitting for Hydrogen Production Using Covalent Organic Framework Catalyst and Ascorbic Acid.....	325
<i>Shohda Makki, Ahmed Abbas, Konstantinos Kakosimos</i>	
521bb Experimental and Theoretical Investigation on Surface Microenvironment Engineered Novel Black Vanadia Towards Visible Light Photodegradation.....	326
<i>Ahmed Badreldin, Ahmed Abdel-Wahab</i>	
521bd A Novel Inexpensive High-Performance Pt-Free Catalyst for Sustainable Hydrogen Fuel Cell	327
<i>Tahmidul Islam, Pabitra Choudhury</i>	
521be Direct Comparisons of Hydrogen Transfer Electrocatalysis across Molecular and Extended Oxides.....	328
<i>Shreya Thakkar, James R. McKone, Christopher E. Wilmer</i>	
521bf Efficient Hydrogen Production Via Surface Reconstruction on Nickel-Molybdenum Electrocatalyst: A DFT Study	329
<i>Hye Bin Yun, Byungchan Han</i>	
521bg A Deep Dive into Dynamic Catalysis: The Impact of Potential Modulation on Formic Acid Electro-Oxidation Efficiency	330
<i>Faviola Villariny-Rosado, Omar Abdelrahman</i>	
521bh Manipulating Inner and Outer Sphere Environments in Zeolites to Control Regioselectivity of Epoxide Methanolysis.....	331
<i>David Potts, Jessica K. Komar, Huston Locht, David Flaherty</i>	
521bi Modeling Active Site Formation of Atomically Dispersed Tungsten Oxide on Silica during Olefin Metathesis	333
<i>Oluwatosin Ohiro, Bryan Goldsmith</i>	
521bj Influence of Cu-CHA Catalyst Composition and Structure on Rates and Selectivities of Catalytic Partial Methane Oxidation to Methanol	334
<i>Andrew Mikes, Rajamani Gounder</i>	
521bk Kinetics of Hydrocarbon Transformations in Zeolite Pores	335
<i>Dipti Bhave, Friederike Jentoft</i>	

521bl Enhanced Catalytic Activity of Gold Nanoparticles in the Small Pore Environment of Mesoporous Silica	336
<i>Zengran Sun, Steven Saunders</i>	
521bm Renewable Activated Carbon Sorbents from Food Waste for the Adsorptive Desulfurization of Liquid Hydrocarbon Fuels	337
<i>Henry Sokol, Julia A. Valla</i>	
521bn Boosting Low-Temperature Dry Methane Reforming on Supported Intermetallic Ni-Zn Nanocatalysts.....	338
<i>Olusola Johnson, Yang He, Babu Joseph, John Kuhn</i>	
521bo Exploiting Properties of Mxenes to Maximize the Metal-Support Interactions (MSI) of Dry Reforming Catalysts	339
<i>Joshua Ighalo, Ahmed Al Mayyahi, Haider Almkhelfe, Placidus B. Amama</i>	
521bp Tandem Catalytic CO ₂ -Assisted Propane Dehydrogenation and Propylene Hydroformylation for Production of Butanal	340
<i>Pin Lim, Marcos Millan</i>	
521bq Process-Level Objectives for Reactor Design and Their Application to the Optimization of Adiabatic Multi-Zone Reactors for Oxidative Coupling of Methane	341
<i>Murtaza Ali Khan, Mamoun Al-Rawashdeh, Patrick Linke</i>	
521br Leveraging Free Radicals for Methane Oxidation and Removal	342
<i>Gang Wan, Arun Majumdar</i>	
521bs Pd Clusters Encapsulated with a Thin TiO _x Layer on Pd-SrTiO ₃ Enable Low-Temperature Semi-Hydrogenation of Acetylene	343
<i>Zhengwen Li, Binhang Yan</i>	
521bt Selective H ₂ Combustion over Alkali Metal-Based Catalysts	345
<i>Elijah Kipp, Niket Kaisare, Aditya Bhan</i>	
521bu Dry Methane Reforming on Ni/Mg/Ce Composite Catalyst with Catalytic Stability.....	346
<i>Jung Hyeok Park, Hyukjun Byun, Kyung-Min Kim, Chang-ha Lee</i>	
521bv Coke-Resistant Single Atom Catalyst for C–H Bond Activation of Methane	347
<i>Naomi Helsel, Keeniya-Gamalage-Gehan De Silva, Sanchari Chowdhury, Pabitra Choudhury</i>	
521bw Application of Silicalite-1 Zeolite Support in Propane Dehydrogenation	348
<i>Xiaoyue Fu, Yingjie Feng, Yue Zhou, Jing Feng, Dongbing Liu</i>	
521bx Plasma-Assisted Approaches for the Direct Conversion of Natural Gas to Liquid Products	349
<i>Deanna Poirier, Jason Hicks</i>	
521by Nonthermal Plasma Activation of Ethane/Nitrogen and Observation of Self-Ordered Nitrogen-Containing Carbon Structures at Sub-Ambient Temperatures	350
<i>Russell J. Clarke, Jason Hicks</i>	
521bz Co-Cation Promoted CH ₄ Oxidation over Pd/SSZ-13 Catalysts.....	351
<i>Jacob Concolino, Tala Mon, Eleni Kyriakidou</i>	
521ca Designing a Concentration-Modulated Microreactor with Integrated Activity Analysis for Dynamic Catalytic Partial Oxidation of Methane.....	353
<i>Fatou Baka Diop, Cameron Armstrong, Geoffrey Tompsett, Andrew R Teixeira</i>	

521cb Engineering Zeolite Catalysts with Tunable Boron Active Sites for Oxidative Dehydrogenation of Propane	354
<i>Chenfeng Huang, Jeffrey D. Rimer</i>	
521cc Enhancing Mass Transport Properties and Catalyst Performance of Low-Dimensional Zeolites	355
<i>Kumari Shilpa, Sambita Choudhury, Jeffrey D. Rimer</i>	
521cd Enhanced Propylene Yield in Olefin Metathesis over Molybdenum and Transition Metal Based Bimetallic Mesoporous Silicates.....	356
<i>Anoop Uchagawkar, Anand Ramanathan, Yongfeng Hu, Bala Subramaniam</i>	
632d Plasma-Assisted Ligand Removal for Improved Catalysis By Pd/SiO ₂	357
<i>Darien Nguyen, Vibin Vargheese, Vinson Liao, Panagiotis Dimitrakellis, Sagar Sourav, Weiqing Zheng, Dionisios Vlachos</i>	
521ce Mercaptan Removal from Natural Gas: An Evaluation of Metal Oxides and Aluminum Silicates As Catalysts.....	358
<i>Gerson Martinez, Mark E. Zappi, William E. Holmes, Emmanuel Revellame, Ling Fei, Rafael Hernandez</i>	
521cf Controlling the Crystallite Shape, Size, and Polydispersity of SSZ-13 Using Stabilizing Agent.....	359
<i>Aditya ., Manjesh Kumar</i>	
521cg Reaction Mechanism and Kinetics of Methanol Carbonylation on Atomically Dispersed ReO _x /SiO ₂ from First Principles.....	360
<i>Nghia Tran, Alexander V. Mironenko</i>	
521ch Zeolites As Selective Catalysts for Cross Aldol Reactions	361
<i>Isaac Ogabiela, Friederike Jentoft</i>	
521ci A DFT-Based Microkinetic Modeling Study to Elucidate the Role of Direct Hydrogen Transfer in Transfer Hydrogenation on Transition Metal Catalysts.....	363
<i>Aojie Li, Srinivas Rangarajan</i>	
521cj Solar-Driven Thermocatalytic Ethylene Oligomerization	364
<i>Aisulu Aitbekova, Magel Su, Matthew Salazar, Harry Atwater</i>	
521cl Using Machine Learning to Model the Enantiospecific Decomposition of Tartaric Acid on Copper Surface Orientations	365
<i>Kareem Abdelmaqsoud, Michael Radetic, Carlos Fernandez-Caban, Zachary Ulissi, John Kitchin, Andrew Gellman</i>	
521cm Trends in C–X Hydrogenolysis: Contrasting Functionalized Alkanes and Aromatics.....	366
<i>Nicole Kragt, Demetrius Williams, Vivian Nguyen, Jalal Tavana, Mohammed Al-Gharrawi, Thomas Schwartz, David Hibbitts</i>	
521cn A Comprehensive Characterization of Catalytic Active Sites in Sodium-Modified Zirconia.....	368
<i>Han Chen, Zhexi Lin, Sai Praneet Batchu, Mengjie Fan, Stavros Caratzoulas, Jingguang G. Chen, Dionisios Vlachos, Raymond Gorte, John Vohs, Omar Abdelrahman</i>	
521co An Advanced Heat Transfer Model for Jacketed Stirred Tank Reactors.....	369
<i>Rachael Lowe, Tariq Mahmud, Peter Heggs, Keeran Ward</i>	
521cp Aldol Condensation of Mixed Oxygenates on TiO ₂ Catalysts	371
<i>Brandon Oliphant, Mathew Rasmussen, J. Will Medlin</i>	

521cq Visible Light Mediated Selective Oxidation of Alcohols Catalyzed By Organic Small Molecules in Batch and Flow	372
<i>Yue Lu, Qingwei Meng</i>	
521cs Effect of Condensed Solvent and Its Organization on Vapor-Phase Alkene Epoxidation with H ₂ O ₂ over Ti-Zeolites	373
<i>Ohsung Kwon, E. Zeynep Ayla, David Potts, David Flaherty</i>	
521ct Kinetic Analysis of Acetone Hydrogenation over Ptsn/SiO ₂	374
<i>Yaqin Tang, Robson Schuarca, Wenlin He, Jesse Bond</i>	
521cu Promotion of Co/SiO ₂ Fischer–Tropsch Catalysts By Manganese and Platinum	375
<i>Fernanda Pimenta, John Kuhn, Babu Joseph</i>	
521cv Microreactors Enabling Safe Ozonolysis Processes with High Space-Time Yields	376
<i>Dominik Polterauer, Christopher Hone, Dominique M. Roberge, Paul Hanselmann, Petteri Elsner, C. Oliver Kappe</i>	
521cw The Noble Metal Promoted V-W/TiO ₂ Catalyst for Simultaneous Removal NO _x and CO on the Dual-Functional Catalyst	377
<i>Jeongtak Kim, Sun-mi Hwang, Hermawan Prajitno, Haewon Jung, Kyuchul Shin, Soon Kwan Jeong, Min Hye Jeong, Kwangsun Yu</i>	
521cy Theoretical Insights into the Photocatalytic PFOA Degradation Mechanism over Boron Nitride.....	378
<i>Yu Chen, Thomas Senftle</i>	
521cz Reactivity of Potential Net-Zero Carbon Fuels on Emissions Control Catalysts.....	379
<i>Sreshtha Sinha Majumdar, Josh A. Pihl</i>	
521da Electrochemical Removal of Perfluoroalkyl Substances from Water By Adsorption and Comprehending Reductive Defluorination.....	380
<i>Mohammad Hasibul Hasan, Ian McCrum</i>	
521db Selective Hydropyrolysis-Prehydrotreating-Hydrotreating Process of Grasses to Produce Fuel Components. Nicepd/SiO ₂ Oxygen Effects in Diesel Emission	381
<i>Roberto Galiasso Tailleur, Irena Panaglia</i>	
521dc Surface Restricted Combustion Synthesis of Ni-Co/SiO ₂ Catalysts for Methane Dry Reforming Reaction.....	382
<i>Afdhal Yuda, Mohd Ali H Saleh Saad, Anand Kumar</i>	
521dd Catalyst Design for Kinetic Modeling of High Yield CNT Synthesis	383
<i>Caleb Bavlnka, Mason Rhue, Laura Alejandra Gomez Gomez, Brian Grady, Steven Crossley</i>	
521de Design of Highly Stable Catalysts from MOF Template for Hydrogen Production in Dry Reforming of Methane	384
<i>Ruth Alli, Nader Mahinpey</i>	
521df Synthesis and characterization of Ceria-supported metal (M)/metal oxide (MO _x)catalysts by novel one pot-chemical vapor deposition (OP-CVD) method.....	385
<i>Amol Pophali, Ryuichi Shimogawa, Lihua Zhang, Gihan Kwon, Anatoly I. Frenkel, Tae Jin Kim</i>	
521dg Dry Methane Reforming for Sustainable Syngas Production By Optimizing Ni-Fe-La Based Catalytic System.....	387
<i>Mohammed Al Mesfer, Mumtaj Shah, Mohd Danish</i>	

521dh Atomic-Scale Insights into Electrocatalyst Structure and Function.....	388
<i>Anthony Hall</i>	
521di Modulation of 0D-2D Hybrids for Improved Efficiency of Pt on Ultra-Thin TiO ₂ Support	389
<i>Prahlad Kumar Routh, Nikhil Tiwale</i>	
521dj Surface Hydroxyl Chemistry of Titania- and Alumina-Based supports: Quantitative Titration and Temperature Dependence of surface Brønsted Acid–Base Parameters.....	390
<i>Tae Yong Yun, Bert Chandler</i>	
521dl Modulating the Physicochemical Attributes of ZSM-5 Using Multivalent Ions-Assisted Synthesis.....	391
<i>M Humam Zaim Faruqi, Manjesh Kumar</i>	
521do Enhanced Photocatalytic Efficiency of Ag-Decorated g-C ₃ N ₄ and NiFe-LDH Heterostructure Under Visible Light Irradiation.....	392
<i>Kamran Alam</i>	
521dp New Synthesis Approaches for Hierarchical Zeolites with Intergrowth Structures.....	393
<i>Zhiyin Niu, Jeffrey Rimer</i>	
521dq A Sustainable Process for Continuous Synthesis and Separation of Silver Nanoparticles Using Segmented Flow with an Aqueous Two-Phase System.....	394
<i>Vamsi Vikram Gande, Rangasamy Savitha, Subramaniam Pushpavanam</i>	
521dr Elucidating the Fluxionality and Dynamics of Zeolite-Confined Au Nanoclusters Using Machine Learning Potentials	396
<i>Chenghan Sun, Siddharth Sonti, Surl-Hee Ahn, Ambarish Kulkarni</i>	
521ds Predicting the Energies of Adsorbate-Saddle Point Interactions Using Machine Learning	397
<i>Matthew S. Johnson, Shinae Kim, Raymundo Hernandez Esparza, David Bross, Judit Zádor</i>	
521du Unlocking the Power of Machine Learning in Catalytic Reaction Optimization	398
<i>César Urbina-Blanco, Daniela Blanco</i>	
521dv Reaction Calorimetry for Adsorption Thermodynamics in Zeolite	399
<i>Ajibola Lawal, Omar Abdelrahman</i>	
521dx Exploring Activity Descriptors in Electrocatalysis of Transition Metal-Oxides Using Computational Tools.....	401
<i>Neha Bothra, Benjamin Comer, Frank Abild-Pedersen, Kirsten Winther, Michal Bajdich</i>	
521dy Developing Predictive Adsorption Energy Descriptors for Unary and Binary Transition Metals By Tailoring Feature Sets for Machine Learning.....	402
<i>Genesis Quiles-Galarza, Aleksandra Vojvodic</i>	
521ea Streamlining Semiautonomous Workflows through Deep Learning for Materials Discovery in the Oxygen Evolution Reaction (OER).....	404
<i>Rohan Sanspeur, John Kitchen</i>	
521eb Are Microkinetic Predictions of (Electrocatalytic) Dynamic Rate Enhancement Robust to Errors in Scaling Relations?	413
<i>Sallye R. Gathmann, Paul J. Dauenhauer</i>	
521ec Plasmonic Photocatalysis By Dynamic Calculations: Mechanisms and Design.....	414
<i>Connor Herring, Matthew Montemore</i>	

521ed Towards Predicting Metal Dynamics, Surface, and Segregation Energies in High Entropy Alloys for Sintering and Catalyst Durability	415
<i>Shyam Deo, Frank Abild-Pedersen</i>	
521ee Unleashing the Power of Hybrid Modeling for Optimization of a Complex Process at Dow.....	417
<i>Reza Haghpanah, Evan Bergman, Brad Metzler, Aayush Singh, David Vickery</i>	
521ef Micro-Kinetics Analysis Based on Partial Reaction Networks to Compare Catalysts Performances for Methane Dry Reforming Reaction	418
<i>Shambhawi Shambhawi, Jana Weber, Alexei A. Lapkin</i>	
521eg Studying Local Hydrodynamics of Co-Current Upflow Packed Bed Reactor (U-PBR) Using Advanced Measurement Techniques	419
<i>Youssef Yatimi, Ahmed Alalou, Muthanna Al-Dahhan</i>	
521ei Wall Effects on Pressure Drop through Randomly Packed Beds of Spherical Catalyst Particles	420
<i>Anthony Dixon</i>	
521ej Dynamic Rate Analysis for Low Frequency Operation of Chemical Reactors.....	422
<i>Austin Morales, Praveen Bollini, Michael Harold</i>	
521ek Quantum Computing Assisted Data-Driven Modeling for Yield Prediction of Naphtha Cracking Process	424
<i>Chonghyo Joo, Seunghyeon Oh, Donggyun Lee, Sayonee Ray, Hyungtae Cho, Il Moon, Junghwan Kim</i>	
521em Interpretable Design of Multimetallic Catalysts for Ammonia Electrooxidation with Deep Learning	425
<i>Shih-Han Wang, Hemanth Pillai, Yi Li, Luke Achenie, Gang Wu, Hongliang Xin</i>	
521en Repurposing Existing Steam Reformers for CO _x -Free Hydrogen Generation through Catalytic Ammonia Decomposition.....	426
<i>Natalia Realpe, Shekhar Kulkarni, Gontzal Lezcano, Salvador Sayas, Natalia Morlanes, Jose Cerillo, Sai P. Katikaneni, Mohammad Rakib, Rosemary Clark, Samuel Clark, Bandar Solami, Ragad F. Aldilaijan, Jorge Gascon, Pedro Castaño</i>	
521eo Programmable Catalytic Ammonia Synthesis and Its Optimization.....	428
<i>Arjun Manoj, Anastasia Georgiou, Georgios Psarellis, Mihalios Kavousanakis, Paul J. Dauenhauer, Ioannis G. Kevrekidis</i>	
521ep Promoting the Enhancement of Low-Temperature Activity and N ₂ Selectivity for NH ₃ -SCR Catalysts Via Changing the Interaction between Fe-Mn Sites.....	429
<i>Weijia Wang</i>	
521er Machine Learning Investigation of Mixed Oxide Supports for Ammonia Synthesis Catalysts	430
<i>Withana A R Jayarathna, Samuel Drummond, Jochen Lauterbach</i>	
154d Hydrothermal Water and Benign Solvent Mixtures for Recycling of Multilayer Plastic Films	431
<i>Madison Reed, Michael T. Timko</i>	
521es Reversible Oxidation of Copper via Chemical Interaction with Carbon Dioxide Investigated by Ambient Pressure X-ray Photoelectron Spectroscopy	433
<i>Haoyi Li, Asmita Jana, Angel T. Garcia-Esparza, Dimosthenis Sokaras, Junko Yano, Ethan Crumlin</i>	

521et Computational Fluid Dynamics Modeling of Industrial Scale Direct Reduced Iron Reforming Process.....	434
<i>Sirisha Parvathaneni, Marcelo Andrade</i>	

CATALYTIC UPCYCLING OF WASTE PLASTICS II: HYDRO-CONVERSION

638a Ru/C Property Insights for Polypropylene Waste Hydrogenolysis	436
<i>Jessie Sun, Pavel Kots, Weiqing Zheng, Dionisios Vlachos</i>	
638b Catalytic Pathways in the Deconstruction of Ethylene Vinyl Alcohol Copolymer.....	437
<i>Christine Oberhausen, Brandon Vance, Dionisios Vlachos</i>	
201h Depolymerization of Polyesters by a Binuclear Catalyst for Plastic Recycling	438
<i>Qikun Hu, Shengbo Zhang, Yu-Xiao Zhang, Zhiqiang Niu</i>	
638d Nickel-Based Catalysts for Low Methane Selectivity in Polyethylene Hydrogenolysis	439
<i>Brandon Vance, Sean Najmi, Pavel Kots, Dionisios Vlachos</i>	
638e Catalytic Hydroconversion of Polyethylene to Gaseous Hydrocarbons on MFI Zeolites Under Mild Conditions.....	440
<i>Jun Zhi Tan, Cole W. Hullfish, Yiteng Zheng, Bruce E. Koel, Michele Sarazen</i>	
638f Using Branched Model Compounds to Understand the Mechanism of C–C Bond Hydrogenolysis of Polyethylene on Catalytic Metal Surfaces	441
<i>Lydia Thies, Andy Simonson, David Hibbitts</i>	
638g Reactivity Investigation and Mechanistic Insights for the Hydrogenolysis of Polyethylene over Silica-Supported Earth-Abundant Cobalt Catalysts	442
<i>Ryan Helmer, Siddhesh Borkar, Manish Shetty</i>	
638h Understanding the Mechanisms of Aromatic Hydrogenolysis and Hydrogenation on Metal Surfaces for Polymer Upcycling Applications.....	444
<i>Andy Simonson, Lydia Thies, David Hibbitts</i>	

CATALYTIC UPCYCLING OF WASTE PLASTICS III: NON-CONVENTIONAL TECHNIQUES

642a Effect of Thermal Pre-Treatment on Pyrolytic Conversion of Polyolefins.....	446
<i>Harish Radhakrishnan, Victor Sanfins Cecon, Lusi A, Md Kaviul Islam, Isabel Coffman, Keith L. Vorst, Xianglan Bai</i>	
642b Microwave Assisted Upcycling Ldpe with Zeolite Supported Catalysts.....	447
<i>Vishal Tuli, Kaushal Parmar, Jianli Hu, Yuxin Wang</i>	
642c Hydroformylation of Plastic Pyrolysis Oils: A New Route to Produce Chemicals from Plastic Waste	448
<i>Houqian Li, Jiayang Wu, Zhen Jiang, Jiaze Ma, Victor Zavala, Clark Landis, Manos Mavrikakis, George Huber</i>	
642d Techno-Economic Analysis and Life Cycle Assessment for the Hydrogenolysis of Waste Plastics.....	449
<i>Geetanjali Yadav, Julie E. Rorrer, Guido Zichittella, Taylor Uekert, Yuriy Román-Leshkov, Gregg Beckham</i>	

642f Plastic Waste Upgrade to Olefins Via Microwave Pyrolysis over Mesoporous Solid Acids.....	450
<i>Esun Selvam, Pavel Kots, Sean Najmi, Dionisios Vlachos</i>	
642g Towards One-Pot Conversion of Polyester Mixtures Using Biocompatible Aqueous Ionic Liquid.....	451
<i>Chang Dou, Hemant Choudhary, Zilong Wang, Nawa Baral, Alexander Holiday, D. Rey Banatao, Corinne D. Scown, Blake Simmons, Jay Keasling, Ning Sun</i>	
642h Chemical Mixed Textile Recycling over Heterogeneous Catalysts	452
<i>Erha Andini, Sunitha Sadula, Dionisios Vlachos</i>	

NITROGEN CHEMISTRY II: NITROGEN THERMOCHEMISTRY

698a Ambient Pressure Carbon-Neutral Ammonia Generation Via a Cyclic Microwave Plasma Process.....	453
<i>Sean Brown, Brandon Robinson, Yuxin Wang, Jianli Hu</i>	
698c Insight into the Dynamic Evolution of $\text{Co}_3\text{Mo}_3\text{n}$ Surface during Ammonia Synthesis.....	454
<i>Shuairan Qian, Binhang Yan, Yi Cheng</i>	
698d DFT Analysis of Speciation and Stability of Surface-Bound Nitrogen Species Under N_2 Plasma Exposure	455
<i>Chang Yan, Garam Lee, David Go, Casey O'Brien, William Schneider</i>	
698e First Principles Membrane Catalyst Co-Design for Low Temperature Ammonia Production.....	456
<i>Pranav Roy, Geet Gupta, Brandon Bukowski</i>	
698f Investigation of Shaped Supports for Ruthenium-Based Catalysts on Ammonia Synthesis	457
<i>Kaveh Shariati, Samuel Drummond, Jennifer Naglic, Jochen Lauterbach</i>	

NEW DEVELOPMENTS IN COMPUTATIONAL CATALYSIS II: DATA-DRIVEN METHODS

696a Predicting Metal Dynamics, Surface, and Segregation Energies in High Entropy Alloys for Sintering and Catalyst Durability	458
<i>Shyam Deo, Frank Abild-Pedersen</i>	
696b Identification of Active Site for Ethane Dehydrogenation on Platinum Catalysts Using Bayesian Analysis: Correction of DFT-Derived Enthalpy and Entropy	460
<i>Mubarak Bello, Olajide Bamidele, Charles Fricke, Gabriel Terejanu, Andreas Heyden</i>	
696c A Probabilistic Microkinetic Modeling Framework for Capturing Spatial Correlations in Complex Catalytic Surface Reactions	461
<i>Aditya Kumar, Abhijit Chatterjee</i>	
696d Design of Active Sites in Bimetallic NO Decomposition Catalysis	462
<i>Joakim Halldin Stenlid, Verena Streibel, Tej Choksi, Frank Abild-Pedersen</i>	
696e Accelerated Phase Diagrams for Metal Carbide Catalysts Under Reaction Conditions Using a Graph-Based Approach	463
<i>Nurul Farhana Binti Abd Ghaffar, Lavie Rekhi, Asmee Prabhu, Luan Q. Le, Pieremanuele Canepa, Wen Liu, Tej Choksi</i>	
696g Machine Learning Approach for Screening Alloy Surfaces for Stability in Catalytic Reaction Conditions	464
<i>Gloria Sulley, Jihun Hamm, Matthew Montemore</i>	

ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS II: CATALYSIS FOR EMISSIONS CONTROL

674a Mechanistic and Structural Transformations of Pt/Al ₂ O ₃ Catalysts during NH ₃ oxidation for NH ₃ Slip Applications	465
<i>Brandon Bolton, Amish Chovatiya, Hanyu Ma, Rohil Daya, Dylan Trandal, Krishna Gunugunuri, Krishna Kamasamudram, William Schneider, Rajamani Gounder</i>	
674c Adsorbate Induced Restructuring of Pt Nanoparticle and Resultant Kinetics for Catalytic Ammonia Oxidation	466
<i>Amish Chovatiya, Brandon Bolton, Hanyu Ma, Rohil Daya, Dylan Trandal, Rajat Subhra Ghosh, Krishna Gunugunuri, Krishna Kamasamudram, Rajamani Gounder, William Schneider</i>	
674d CO and C ₃ H ₆ oxidation on Pd-Based Three-Way Catalysts: Effects of Loading and Aging Protocols on Particle Size Calculation.....	467
<i>Silvia Marino, Natalia Diaz Montenegro, Kevin Gu, Wei Li, William Epling</i>	
674e Hydrothermal Stability and so ₂ Poisoning Resistance of High Silica Pd/SSZ-13 Minicores for CH ₄ Oxidation	468
<i>Tala Mon, Eleni Kyriakidou</i>	
674f Improved Low-Temperature Catalytic Combustion of Methane over Pd in High-Silica Chabazite Zeolites	470
<i>Jingzhi Liu, Tala Mon, Robson Schuarca, Jesse Bond, Eleni Kyriakidou, Viktor Cybulskis</i>	
674g Intra-Catalyst CH ₄ Oxidation Pathways of Three Way Catalysts and Implications on NO _x Conversion Profiles for a Natural Gas Vehicle Exhaust Under Lambda Dithering	472
<i>Dhruba Jyoti Deka, Calvin Thomas, Josh A. Pihl, William P. Partridge</i>	
674h Influence of Engine Oil Derived Chemical Species on the Performance of Cu-SSZ-13 SCR Catalysts	473
<i>Poonam Rani, Huifang Shao, Elisabetta Bonaglia, Giovanni Bevilacqua, William Epling</i>	

THERMAL AND THERMOCATALYTIC BIOMASS CONVERSION AND BIOREFINING II

704a Tunable Cellulose Fast Pyrolysis Via Noncovalent Interactions Induced By Molten Plastics.....	474
<i>Fuat Sakirler, Mihriye Doga Tekbas, Hsi-Wu Wong</i>	
704b Experimental Studies and Kinetic Modeling of Co-Pyrolysis of Biomass and Plastic Wastes with the Combined Scheme of Kinetics and Machine Learning Method	475
<i>Hui Liu, Hesham Alhumade, Ali Elkamel</i>	
704c Evaluating Tungsten Doped Molybdenum Carbide for the Selective Hydrodeoxygenation of Real Bio-Oil: A DFT Study Using Lignin and Carbohydrates Derived Bio-Oil Components	476
<i>Sagar Bathla, Samir H. Mushrif</i>	
704d Thermocatalytic Conversion of Wet Waste to Sustainable Aviation Fuel and Chemical Precursors	477
<i>Jacob Miller, Mayadhin Al Abri, Nabila Huq, Jim Stunkel, Derek Vardon</i>	
704g Green Fuel from Hydrotreated Vegetable Oil Using Ni-Fe/Zelite Y Catalysts.....	478
<i>Tzu-Yang Juang, Bing-Hung Chen</i>	

704f Ionothermal Carbonization of Agricultural Waste into Porous Biochar for CO ₂ Capture	480
<i>Sanphawat Phromphithak, Nakorn Tippayawong, Thossaporn Onsree, Kenneth Roberts, Jochen Lauterbach</i>	

CATALYST DESIGN, SYNTHESIS, AND CHARACTERIZATION II: CONTROL OF CATALYTIC SITE SPECIATION AND DISTRIBUTION

594a Rigorous Oxidation State Assignment for Ga Catalysts Using Theory-Informed X-Ray Absorption Spectroscopy Signatures from Well-Defined Ga(I) and Ga(III) Compounds	481
<i>Simon Bare, Fernando Vila, Jason A. Chalmers, Susannah L. Scott</i>	
594b Influence of the Crystallite-Scale Spatial Distributions of Framework Al Sites in MFI Zeolites on Propene Oligomerization Catalysis	482
<i>Ricem Diaz Arroyo, Rajamani Gounder</i>	
594c Ion Exchange and Chemical Titration for Aluminosilicate Paired Site Quantification.....	483
<i>Ajibola Lawal, Omar Abdelrahman</i>	
594d Characterization of the Structural Changes of Tin Sites throughout the Life Cycle of Sn-β Prepared By Post-Synthetic Methods	485
<i>Edgard Lebron Rodriguez, Faysal Ibrahim, Isabel Hortal-Sánchez, Jadiel López-González, Angela Montano-Herazo, Nelson Cardona Martinez, Ive Hermans</i>	
594e Elimination of Acetylene from Ethylene Using Pd ₁ @Zeolite.....	486
<i>Yiqi Xu, Adam Holewinski, J. Will Medlin</i>	
594f Designing Ti-Zeolites with Gradients in Heteroatom Composition for Improved Olefins Epoxidation	487
<i>Chenfeng Huang, Ohsung Kwon, David Flaherty, Jeffrey Rimer</i>	
594g Constraining Local Environments in Oxide Catalysts.....	488
<i>Justin Notestein, Kenton Hicks, Katie Chase, Omar Farha</i>	
521dt Non-Mean Field Approaches for Surface Catalysis: Analytical Description of Adsorbate-Adsorbate Interactions.....	489
<i>Purva Paranjape, Jeffrey Greeley</i>	

CATALYST DESIGN, SYNTHESIS, AND CHARACTERIZATION III: MODIFYING DOMAIN SIZE AND TRANSPORT PROPERTIES

607a Effects of Domain Size and Support Composition on the Reactivity and Reducibility of Oxide-Supported Tungsten Oxide Clusters	490
<i>Anukriti Shrestha, Konstantin Mamedov, Robert J. Davis, Christopher Paolucci</i>	
607b Steering the Molecular Diffusion Pathway of H-ZSM-5 Zeolites to Regulate Their Catalytic Performances	491
<i>Liu Xiaoliang, Teng Jiawei, Yangdong Wang, Zhou Jian, Zaiku Xie</i>	
607c Ethylene Epoxidation over Shape-Selective Silver-Based Catalysts	493
<i>Kaveh Shariati, Jochen Lauterbach</i>	
607e How Structural Evolution during Strong Metal Support Phenomena Influences Reaction Rates and Selectivity	494
<i>Luan Q. Le, Hui Ling Tan, Lavie Rekhi, Mingwu Tan, Roong Jien Wong, Wen Liu, Tej Choksi</i>	

607f Highly Active Nanoporous Solid Base MgO Catalyst Derived from Mg-MOF-74 Towards Knoevenagel Reaction.....	496
<i>Mahdi Niknam, Christian Geci, Brian G. Frederick, Thomas Schwartz</i>	
607g Design Strategies for Improved Pairwise Addition of Parahydrogen to Unsaturated Compounds over Heterogeneous Catalysts	498
<i>Helena Hagelin Weaver, Hanqin Zhao, Michelle Lapak, Nicole Virgilio, Li-Yin Hsiao, Diana Choi, Clifford R. Bowers</i>	
607h Role of Confinement Effects for Zn Deposition Via Polymer Additives Onto Acid Catalysts.....	499
<i>Ana Carolina Jerdy, Ron Abbott, Masud Monwar, Miguel Gonzalez Borja, Lance Lobban, Steven Crossley</i>	

CATALYST DESIGN, SYNTHESIS, AND CHARACTERIZATION IV: EXPERIMENTAL AND COMPUTATIONAL CATALYST CHARACTERIZATION

616a Operando XAS Characterization of $Mn_{0.1}Cu_xCo_{2.9-x}O_4$ Direct NO _x Decomposition Catalysts	500
<i>Jiyun Hong, Kimber L. Stamm Masias, Jorge Perez-Aguilar, Torin C. Peck, Adam Hoffman, Charles A. Roberts, Simon Bare</i>	
616b Spectroscopic Characterization of Inverse Catalysts.....	501
<i>Sagar Sourav, Yurong Wu, Jiahua Zhou, Alfred Worrad, Stavros Caratzoulas, Weiqing Zheng, George Tsilomelekis, Dionisios Vlachos</i>	
616c Pt ₃ Zn ₁ and Pt ₁ Zn ₁ Intermetallic Nanocatalysts Synthesis and Characterization	502
<i>Zhuoran Gan, Zheng Lu, Muntaseer Bunian, Larissa Lagria, Christopher L. Marshall, R. Michael Banish, Sungsik Lee, Yu Lei</i>	
616d Chemical Engineering at the Stanford Synchrotron Radiation Lightsource (SSRL) XAS Beamlines	503
<i>Jorge Perez-Aguilar, Simon Bare, Adam Hoffman</i>	
616e Ab Initio Molecular Dynamics Spectra for Characterization of Hydrated Supported Metal Oxide Catalysts.....	504
<i>Alfred Worrad, Sagar Sourav, Stavros Caratzoulas, Dionisios Vlachos</i>	
616f Catalytic Decomposition of Tritiated Ammonia As a By-Product of Nuclear Fusion.....	505
<i>Jennifer Naglic, Jochen Lauterbach</i>	
616g Understanding the Influence of Metal Composition on Aldol Condensation Reactions over Mg _x AlO _y -Type Materials Via Combined Experimental and Computational Investigations.....	506
<i>Ho Yi Lam, Davi Petrolini, Prashant Deshlahra, Nathaniel Eagan</i>	
616h Using XPS to Tune Catalyst Design and Performance	507
<i>Danielle Covelli, Shuo Cao</i>	

CATALYST DESIGN, SYNTHESIS, AND CHARACTERIZATION V: TAILORING BULK AND SURFACE STRUCTURES

625a Promoting Pdo Formation Via Pre-Exposure to Ambient Moisture.....	508
<i>Tala Mon, Jacob Concolino, Junjie Chen, Eleni Kyriakidou</i>	

625b Impregnation of Koac on PdAu/SiO ₂ Causes Pd-Acetate Formation and Metal Restructuring	510
<i>Hunter P. Jacobs, Welman C. Elias, Kimberly N. Heck, David P. Dean, Justin J. Dodson, Wenqing Zhang, Jacob H. Arredondo, Christian J. Breckner, Kiheon Hong, Christopher R. Botello, Laiyuan Chen, Sean G. Mueller, Steven R. Alexander, Jeffrey T. Miller, Michael Wong</i>	
625c Generation of Abundant Oxygen Vacancies in Fe Doped δ-MnO ₂ By a Facile Interfacial Synthesis Strategy for Highly Efficient Catalysis of VOCs Oxidation	511
<i>Yang Shuo</i>	
625d Propane Dehydrogenation on Different Platinum Surfaces and in the Presence of Al ₂ O ₃ ALD Layer.....	512
<i>Sumandeep Kaur, Hoan Nguyen, Stuart Helikson, Liney Arnadottir</i>	
625e Efficient Cu-Based Catalysts for CO ₂ Hydrogenation to Methanol: An Exsolution Strategy with CuAl ₂ O ₄ As Precursor	513
<i>Xiaohang Sun, Binhang Yan</i>	
625f Tunable Palladium Catalyst Using Organically Modified Silica As a Scaffold for Aqueous Phase Phenol Hydrogenation.....	515
<i>Snehal Patil, Anagha Hunoor, Paul Edmiston, Umit Ozkan</i>	
625g Tuning Palladium Hydride Formation with Hypophosphite: A Sustainable Hydrogen Source for Fuel Cells	516
<i>Sihe Zhang, Michaela Burke Stevens, Adam Nielander, Thomas Jaramillo</i>	
625h Optimizing the Properties of Ti ₂ N Mxene through Decoupling Surface and Bulk Structure and Phenomena	517
<i>Ray Yoo, Denis Johnson, Abdoulaye Djire</i>	

CATALYST DESIGN, SYNTHESIS, AND CHARACTERIZATION VI: CATALYST SYNTHESIS AND PREPARATION

632b Fast and Continuous Flow Hydrothermal Synthesis of MoVNbTeO _x Mixed Metal Oxides in Micro Droplet — Large-Scale Accessibility of MoVNbTeO _x Catalysts	518
<i>Yuxin Chen, Yuting Wu, Binhang Yan, Yi Cheng</i>	
632c Tuning Gold Nanoparticle Surface Site Accessibility and Electronic State Using Organic Ligands for Oxidation and Reduction Catalysis	519
<i>Sayed Abu Sufyan, Michael Nigra</i>	
632e Enhancing Light Olefin Production from Syngas Via Indium-Promoted Iron Catalysts	520
<i>Yang He, Hanzhong Shi, Olusola Johnson, Babu Joseph, John Kuhn</i>	
632f Enhancing the Activity and Stability of Nickel-Supported Catalysts for Dry Reforming of Methane Using Halloysite Nanotubular Clay As a Support	521
<i>Ahmed Abotaleb, Dema Al-Masri, Alaa AlKhateb, Alessandro Sinopoli</i>	
632g Directing Reaction Pathways on Supported Metal Catalysts with Low-Density Self-Assembled Monolayers	522
<i>Zachary Blanchette, Daniel K. Schwartz, J. Will Medlin</i>	
632h Hydrodechlorination of Chloro-Organic Contaminants in Drinking Water: Design of Bimetallic Alloy Catalysts.....	523
<i>Chaitra Shenoy, Tuhin Suvra Khan, Shelaka Gupta, M. Ali Haider</i>	

CO2 UPGRADING II: ELECTROCHEMICAL APPROACHES

650b First Principles Study of Copper Cathodic Corrosion during CO ₂ rr.....	524
<i>Hori Pada Sarker, Frank Abild-Pedersen</i>	
650c Enhanced Electrochemical CO ₂ Reduction Using DNA-Based Nanomaterials	525
<i>Gang Fan, Ariel Furst</i>	
650d Interfacial Engineering of Metal/Support Heterostructures for CO ₂ Electro-Reduction to C ₁ Products and Beyond.....	526
<i>Lavie Rekhi, Luan Q. Le, Asmee Prabhu, Kah Meng Yam, Tej Choksi</i>	
650e Continuous Gas-to-Liquid Conversion for Carbon-Efficient Electroreduction of CO ₂	527
<i>Chengao Zhou, Hao Shen, Chao Wang</i>	
650h Efficient Formation of C-N Bond and Multi-Carbon Liquid Products in Electrochemical CO Conversion.....	528
<i>Haocheng Xiong, Qi Lu, Bingjun Xu</i>	

CO2 UPGRADING III: ALTERNATIVE APPROACHES

654a Organic-Inorganic Interface Enhanced CO ₂ Capture and Conversion.....	529
<i>Mingyu Wan, Zhiyong Gu, Hsi-Wu Wong, Fan Shi, Fanglin Che</i>	
654b Direct Synthesis of Branched Hydrocarbons from CO ₂ Hydrogenation over Composite Catalysts in a Single Reactor	531
<i>Anh To, Martha A. Arellano-Treviño, Daniel Ruddy, Connor P. Nash</i>	
654c Tandem Electrocatalytic and Thermocatalytic Reactors for CO ₂ Conversion to BTEX Aromatics	532
<i>Samay Garg, Zhenhua Xie, Alexandria Lam, Jingguang G. Chen</i>	
654d Synthesis of Aromatic Compounds Via CO ₂ hydrogenation on H-Fe-ZSM-5 / ZnO-ZrO ₂ Tandem Catalysts.....	533
<i>Dhrumil Shah, Iman Nezam, Christopher Jones</i>	
654e CO ₂ Upgrading into Solid Carbon-Based Nanomaterials: From Reduced Graphene Oxide to Novel Materials	534
<i>Ahmed Badreldin, Ahmed Abdel-Wahab</i>	
654g Unveiling the Difference between CO ₂ and CO Reduction of Cobalt Phthalocyanine on CNT.....	535
<i>Haozhou Yang, Lei Wang</i>	
654h Effect of Proximity on Hydrocarbon Selectivity in the Tandem Hydrogenation of CO ₂ Utilizing Zeolite-Tailored Bifunctional Catalyst	536
<i>Fatima Mahnaz, Jasan Robey Mangalindan, Manish Shetty</i>	

CO2 UPGRADING IV: ALTERNATIVE APPROACHES II

655a Capture and Reuse of Carbon Dioxide Using Electrochemical Reduction to Produce Carboxylic Acids	537
<i>Philip Cox, Vincent Storhaug</i>	

655b Investigation of the Role of Supports for Ni Based CO ₂ Methanation	538
<i>Majed Alam Abir, Joseph Harrah, Rachel Phillips, Madelyn Ball</i>	
655c Carbon Dioxide Conversion into Polycarbonate Diols: A Parametric Study	539
<i>Swarom Kanitkar, Pranjali Muley, Wu Zhang, Daniel Haynes</i>	
655d Aging Studies of Dual Functional Materials for Direct Air Capture with in Situ Methanation Under Simulated Ambient Conditions: Ru Thrifiting for Cost Reduction.....	540
<i>Yuanchunyu Lin, Monica Abdallah, Huan Sheng, Robert Farrauto</i>	
655e Visualizing the Effect of Reaction Parameters and Catalyst Configuration for Tandem Hydrogenation of CO ₂ to Gasoline-Range Hydrocarbons.....	542
<i>Fatima Mahnaz, Jasan Robey Mangalindan, Manish Shetty</i>	
655f A Scalable Integrated Solar Device for the Autonomous Production of Synthetic Fuel.....	544
<i>Angela R. A. Maragno, Gregory Cwicklinski, Matheron Muriel, Jean-Marc Borgard, Adina Morozan, Jennifer Fize, Michel Pellat, Christine Cavazza, Vincent Artero, Sophie Charton*</i>	
655h CO ₂ Heterogeneous Catalytic Hydrogenation to Formic Acid over Ru-Based Catalyst: Kinetics and Reactor Optimization.....	546
<i>Tesfalem Atsbha, Taeksang Yoon, Ali Cherif, Arash Esmaeili, Mohammed Atwair, Chul-Jin Lee</i>	

CO₂ UPGRADING V: MECHANISTIC INSIGHT II

658a Significantly Improved Efficiency of CO ₂ /CO Electroreduction to Value-Added Liquid Fuels Via Rational Catalyst Design.....	547
<i>Jing Li, Hailiang Wang</i>	
658b Enhancing the CO ₂ Hydrogenation to Higher Alcohols By Potassium Promotion of Cocu Catalysts	548
<i>Caiqi Wang, Norbert Kruse, Hongfei Lin</i>	
658c Tuning the Hydrogenation of CO ₂ to CH ₄ over Mechano-Chemically Prepared Palladium Supported on Ceria.....	549
<i>Juan Jimenez, Maila Danielis, Ning Rui, Jorge Moncada, Luis E. Betancourt, Alessandro Trovarelli, Jose A. Rodriguez, Sara Colussi, Sanjaya D. Senanayake</i>	
658d Reverse Water Gas Shift Reaction of Transition Metal-Promoted Cu/Metal Oxide Catalyst for Enhancing Reaction Rate	550
<i>Hyukjun Byun, Jung Hyeok Park, Kyung-Min Kim, Chang-ha Lee</i>	
658f Boosting Ethanol Selectivity in Electrocatalytic CO ₂ Reduction Reaction through Confinement of Intermediates in Au/Cu Tandem Catalyst	551
<i>Yesol Kim, Sojung Park, Woo-Bin Jung, Hee-Tae Jung</i>	
658g Theoretical Insights into Selectivity Differences to Form Ethylene and Ethanol in the Electrocatalytic Reduction of CO ₂ over Cu Electrodes	552
<i>Huy Nguyen, Nishant Sinha, Matthew Neurock</i>	
658h Functionalized Ag with Thiol Ligand to Promote Effective CO ₂ Electroreduction.....	553
<i>Junmei Chen, Lei Wang</i>	

DATA SCIENCE AND MACHINE LEARNING APPROACHES TO CATALYSIS II: CATALYTIC MATERIALS DESIGN

662a Machine Learning for Homogeneous Open-Shell Transition Metal Catalyst Discovery.....	554
<i>Heather Kulik</i>	
662b Intermetallic Catalyst Discovery for Selective Hydrogenation Reactions.....	555
<i>Jin LI, Angela Nguyen, Unnatti Sharma, Rushi Gong, Griffin A. Canning, Robert Rioux, Zikui Liu, Zachary Ulissi, Michael Janik</i>	
662c Integrating Experimental and Theoretical Data for High Quality Predictions of Material Performance Towards Electrochemical Reactions.....	557
<i>Shyam Deo, Gaurav A. Kamat, Melissa E. Kreider, Michaela Burke Stevens, Kirsten Winther, Johannes Voss</i>	
662d Machine Learning Electron Density for Chemical Property Predictions in Catalysis	559
<i>Ethan Sunshine, Muhammed Shuaibi, Zachary Ulissi, John Kitchin</i>	
662e Predicting the Adsorption Energies of Cyclic Hydrocarbons Adsorbed on Bimetallic Nanoclusters Using Gaussian Process Regression	560
<i>Chuhong Lin, Uzma Anjum, Chak Sing Bryan Lee, Asmee Prabhu, Tej Choksi</i>	
662f Improving the Accuracy of ML-Models for Catalysis through Bulk Electronic Structure Descriptors.....	561
<i>Kirsten Winther</i>	
662g Clarifying Trust of Materials Property Predictions Using Neural Networks with Distribution-Specific Uncertainty Quantification	562
<i>Cameron Gruich, Varun Madhavan, Yixin Wang, Bryan Goldsmith</i>	

DATA SCIENCE AND MACHINE LEARNING APPROACHES TO CATALYSIS III: DATA WORKFLOWS AND AUTOMATION

663a Self-Driving Catalysis Lab: Research Acceleration in Homogeneous Catalysis Enabled By Autonomous Flow Reactors	564
<i>Milad Abolhasani</i>	
663b Redefining Structure-Property Relationships for Accelerating Decarbonization	565
<i>Andrew White, Marc Porosoff</i>	
663c Catalysts Discovery Via Curated Computational Databases: Past, Present and Future of Catalysis- Hub.Org	566
<i>Michal Bajdich, Kirsten Winther, Neha Bothra</i>	
663d Data-Driven Models for Catalyst Synthesis and Stability	567
<i>Daniel Schwalbe-Koda</i>	
663e Active Learning Workflow for Discovery of Stable Ternary Alloys from Binary Alloy Data	568
<i>Gaurav Deshmukh, Noah J. Wichrowski, Nikolaos Evangelou, Pushkar Ghanekar, Siddharth Deshpande, Ioannis G. Kevrekidis, Jeffrey Greeley</i>	

ELECTROCATALYSIS AND PHOTOCATALYSIS I: ELECTROCATALYTIC CO₂ AND CO REDUCTION

664a Intercepting Elusive Intermediates in Cu-Mediated CO Electrochemical Reduction with Alkyl Species.....	569
<i>Jing Li, Bingjun Xu</i>	
664b Correlating CO Coverage and CO Electroreduction on Cu Via High-Pressure in Situ Spectroscopic and Reactivity Investigations	570
<i>Jiajie Hou, Qi Lu</i>	
664c Automated Platform for Quantitative Kinetic Analysis of CO ₂ Electroreduction Mechanisms at Immobilized Metal Tetrapyrroles	571
<i>Joy Zeng, Vineet Padia, Joseph Maalouf, Aditya Limaye, Alexander Liu, Michael Yusov, Ian Hunter, Karthish Manthiram</i>	
664d Controlling Electrochemical Reactivity By Tuning the Activity of Water	572
<i>Anthony Hall</i>	
664e Asymmetrical C–C Coupling for Electroreduction of CO on Bimetallic Cu–Pd Catalysts	573
<i>Hao Shen, Yunzhe Wang, Tim Mueller, Chao Wang</i>	
664f The Role of Surface Roughening in Improving the Selectivity of Copper for CO ₂ Electroreduction	574
<i>Joakim Halldin Stenlid, Joseph Gauthier, Alexis T. Bell, Martin Head-Gordon, Frank Abild-Pedersen</i>	
664g Selective Electrochemical Reduction of NO ₃ ⁻ and CO ₂ to Urea on Silver Gas Diffusion Electrode.....	575
<i>Nishithan Balaji Chidambara Kani, Ishita Goyal, Meenesh R Singh</i>	

ELECTROCATALYSIS AND PHOTOCATALYSIS V: PHOTOELECTROCATALYSIS AND PHOTOCATALYSIS

668a Balancing Charge Carrier Kinetics and Photo-Absorption Capacity through Strain Engineering to Maximize Photocatalysis Under Visible-Light.	576
<i>Rohit Pal, Ramin Farnood</i>	
668b A Tale of Two Cities - TiO ₂ Impregnated Mesoporous Silica Nanoparticles and TiO ₂ Coated Thin Films As Photocatalysts in Wastewater Treatment.....	578
<i>Deepa Khandekar, Rajdip Bandyopadhyaya</i>	
668c Exploring the Performance Limits of Nanoscale Electrocatalysts on Planar Semiconductor Light Absorbers for the Oxygen Evolution Reaction	580
<i>Aarti Mathur, John Hemmerling, Suljo Linic</i>	
668d An Enhanced Generation of Singlet Oxygen through the Use of Au Bipyramids/SiO ₂ core-Shell Nanoparticles for Photocatalysis	581
<i>Carlos Mendoza, Denis Chateau, Anthony Desert, Carlos Paez, Noemie Emmanuel, Lhoussain Khrouz, Cyrille Monnereau, Laurent Dreesen, Jean-Christophe Monbaliu, Stephane Parola, Benoit Heinrichs</i>	
668e Experimental and Modeling Analysis of the Role of Insulating Layers on the Performance of Metal-Insulator-Semiconductor Photoelectrocatalysts for Solar Water Splitting	582
<i>Ahmet Sert, Aarti Mathur, John Hemmerling, Suljo Linic</i>	

668f Interfacial Engineering of Au/Cu _x O _y H _z Heterostructures for Efficient Photocatalytic CO ₂ Reduction: Insights from Theoretical Approaches	583
<i>Pooja Basera, Marija Zoric, Hori Pada Sarker, Frank Abild-Pedersen, Amy Cordones-Hahn, Michal Bajdich</i>	
668g Molecular Additives Steer Selectivity of CO ₂ Photoelectrochemical Reduction over Gold Nanoparticles on Gallium Nitride.....	584
<i>Aisulu Aitbekova, Harry Atwater</i>	

ELECTROCATALYSIS AND PHOTOCATALYSIS IV: OXYGEN ELECTROCATALYSIS

667a Synthesis, Activity Testing, and Soft X-Ray Spectroscopy of Nickel-Iron (Oxy)Hydroxide Oxygen Evolution Electrocatalysts	585
<i>Raheleh Daneshpour, Ragini Sengupta, Constantin Wansorra, Dirk Hauschild, Ralph Steining, Lauren F. Greenlee, Clemens Heske, Michael Janik, Lothar Weinhardt, Ezra Clark</i>	
667b Tuning the Bulk Composition of Pt-Based High-Entropy Alloys for Improved Oxygen Reduction Activity.....	586
<i>Gaurav Deshmukh, Fei Xu, Qingzhe Xin, Canhui Wang, Chao Wang, Jeffrey Greeley</i>	
667c Understanding Activation in Mixed Metal Oxides and High Entropy Spinel Oxides for Oxygen Evolution Reaction	587
<i>Michal Bajdich, Md Delowar Hossain, Jihyun Baek, Kirsten Winther, Xiaolin Zheng</i>	
667d A Structural and Mechanistic Study of Electrochemical Ozone Production on Doped Tin Oxide Electrodes	588
<i>Rayan Alaufey, Maureen Tang</i>	
667e Catalytic Performance and Material Stability Trends of Iridium 5+ Materials for Acidic Water Oxidation.....	589
<i>Jane Edgington, Linsey Seitz</i>	
667f An Ab-Initio Molecular Dynamics Study of the Metal-Water Interface for ORR Activity in Alkaline Media.	590
<i>Ara Cho, Jeong Woo Han, Frank Abild-Pedersen</i>	
667g Designing Single Site Catalysts for the Two-Electron Oxygen Reduction Reaction By Tailoring Environments Beyond the Binding Site.....	591
<i>Tej Choksi, Xiaogang Li, Luan Q. Le, Kah Meng Yam, Xin Wang</i>	

ELECTROCATALYSIS AND PHOTOCATALYSIS VI: THE ROLE OF MICROENVIRONMENTS IN ELECTROCATALYSIS

669a Electrifying Industrial Chemistry: Controlling the Electrocatalytic Transformation of Alcohols and Alkanes to Valuable Products.....	592
<i>Marcel Schreier, Christine Lucky</i>	
669b How the Electrochemical Medium Influences Surface Catalytic Activity	593
<i>Joaquin Resasco</i>	
669c An Alternative Electrode Model for Understanding Reductive Microenvironments	594
<i>Michael Tang, Ara Cho, Hyeonjung Jung, Frank Abild-Pedersen</i>	

669e Descriptors for Electrochemical Anion Adsorption and the Mechanism of Electrocatalytic Glycolic Acid Oxidation	595
<i>Ian McCrum, Mohammad Hasibul Hasan</i>	
669f Proton Transfer and Acidity at the IrO ₂ -Water Interface from Deep Potential Molecular Dynamics Simulations.....	596
<i>Abhinav Sankara Raman, Annabella Selloni</i>	
669g Re-Structuring of Interfacial Water into Strongly Hydrogen Bonded “Ice-like” Structures As the Unifying Descriptor for Improving Sluggish HOR/HER in Alkaline Electrolyte	597
<i>Nicholas Oliveira, Yushan Yan</i>	

ELECTROCATALYSIS AND PHOTOCATALYSIS II: ELECTROCATALYTIC MATERIALS

665a Decorated Steps As a Novel Alloy Electrocatalyst	599
<i>Onyinyechukwu Njoku, Ian McCrum</i>	
665b FTIR Spectroelectrochemistry: Optimization of Experimental Setup	600
<i>Sergey Shilov</i>	
665c Metal-Metal, Metal-Oxide and Oxide-Oxide Interfaces in Electrochemical Energy Conversion	601
<i>Zhenhua Zeng, Jeffrey Greeley</i>	
665d Unraveling the Effect of Electrochemical Pre-Treatment on the Structure and Performance of the Electrocatalysts.....	602
<i>Aniket Sandip Mule, Kevin Tran, Ashton M. Aleman, Gaurav A. Kamat, Michaela Burke Stevens, Thomas Jaramillo</i>	
665e Laser-Made Mixed-Metal Hydroxide Nanocatalysts for Selective Electrooxidation of Toluene to Benzyl Alcohol.....	603
<i>Astrid Muller</i>	
665f Effect of Delamination Chemistry on Electrochemical Reduction Reactions of Ti ₄ N ₃ nitride Mxene.....	604
<i>Eugenie Marie Pranada, Bright Ngozichukwu, Denis Johnson, Ray Yoo, Abdoulaye Djire</i>	
665g Phase-Dependent Promoting Effect of Surface Oxygen on Molybdenum Carbide Catalysts during Formic Acid Electrooxidation	605
<i>Ankit Kumar Gautam, Alexander V. Mironenko</i>	

FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE II: C1 CATALYSIS

676a Impact of Pt Nuclearity on CO ₂ Reduction and Aldol Condensation Reactions.....	606
<i>Honghong Shi, Shiva Murali, Fan Lin, Yubing Lu, Yifeng Zhu, Linxiao Chen, John L. Fulton, Libor Kovarik, Mark Bowden, Johannes Lercher, Yong Wang, Huamin Wang, Oliver Gutiérrez-Tinoco</i>	
676b Contrasting Methylating Agents (CH ₃ XH _n , X={N, P, O, S, F, Cl}) for Solid-Acid Catalyzed Reactions to Re-Examine Acid Strength and Confinement Effects.....	607
<i>Samuel Mercer, Hansel Montalvo-Castro, David Hibbitts</i>	
676c Characterization of the Structural Evolution of Mo-MFI for Methane Dehydroaromatization Reaction-Regeneration Cycles	608
<i>Angel Santiago-Colón, Rajamani Gounder</i>	

676d Catalytic Trends for CO ₂ Hydrogenation Reactivity and Selectivity on Transition Metals.....	609
<i>Michelle Nolen, Stephanie Kwon, Carrie Farberow</i>	
676e Ru or Fe? Understanding Trends in C–H Activation Catalysis with High-Throughput Screening	610
<i>Husain Adamji, Ilia Kevlishvili, Aditya Nandy, Yuriy Román-Leshkov, Heather Kulik</i>	
676f The Fe Catalyzed Boudouard Reaction: Mechanism, Rate Limiting Steps, and Structural Evolution of the Fe Catalyst	611
<i>Jordan Finzel, Phillip Christopher</i>	
676g Trends in Methanol Decomposition over Supported Metal Catalysts	612
<i>Atharva Burte, Omar Abdelrahman, Ashwin Ramasubramaniam</i>	
676h Effects of Site Distribution and Dynamic Character of Atomically Dispersed Catalysts on CO Oxidation Kinetics.....	613
<i>Selin Bac, Nicholas Humphrey, Shaama Mallikarjun Sharada</i>	

FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE III: CATALYSIS OVER METALS

677a Controlling C–O, C–C, and C–H Bond Scission Pathways on Metal-Modified Molybdenum Nitride Catalysts	614
<i>William N. Porter, Hilda Mera, Wenjie Liao, Zhexi Lin, Ping Liu, John Kitchin, Jingguang G. Chen</i>	
677b In Situ/Operando Spectroscopic, Computational, and Kinetic Study of Ethanol Partial Oxidation on Au/TiO ₂	616
<i>Alejandra Torres-Velasco, Bhagyesh Patil, Hongda Zhu, Yue Qi, Simon G. Podkolzin, Juan Bravo-Suarez</i>	
677c Wet Metal-Support Interfaces Control Paths of H ₂ and O ₂ Activation over Au Nanoparticles.....	617
<i>Jason S. Adams, Haoyu Chen, Sucharita Vijayaraghavan, Tomas Ricciardulli, Abinaya Sampath, David Flaherty</i>	
677d Catalytic Hydrogenation of Arenes on Densely-Covered Pt Nanoparticles: Kinetically-Relevant Steps and Unusual Temperature Effects on Turnover Rates.....	619
<i>Ari Fischer, Enrique Iglesia</i>	
677e Optimizing Adsorption on Gold Surface in the Small Pores of Mesoporous Silica	620
<i>Zengran Sun, Anthony Savoy, Megan Hawkins, Di Wu, Yong Wang, Steven Saunders</i>	
677f Elucidating the Influence of Water-Saturated Cs on Phenol Tautomerization.....	621
<i>Naseeha Cardwell, Isaac Onyango, Yong Wang, Jean-Sabin McEwen</i>	
677g Spectroscopic, Theoretical, and Data Science Insights into Selective Oxygen Species for Ethylene Epoxidation over Ag Supported on α -Al ₂ O ₃ Catalysts	622
<i>Shawn Lu, Jin-Xun Liu, Shiuan-Bai Ann, Suljo Linic</i>	
677h Classification of Adsorbed Hydrocarbons Based on Surface Site Stabilities	623
<i>Shyama Charan Mandal, Frank Abild-Pedersen</i>	

FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE IV: ELECTROCATALYSIS

678a How Metal/Support Heterostructures Influence the Design Principles and Limiting Potentials for the Oxygen Reduction Reaction	624
<i>Asmee Prabhu, Kah Meng Yam, Lavie Rekhi, Luan Q. Le, Tej Choksi</i>	
678b Mechanistic Insights into the Influence of the Electrode Surface in the Selective Alcohol Oxidation of Primary Benzyl Alcohols.....	625
<i>Kaida Liu, Enqi Feng, Mayank Tanwar, Qiwei Jing, Kevin Moeller, Matthew Neurock</i>	
678c Monitoring the Electrocatalytic Activity and Material Stability of Cobalt in Acidic Media during Oxygen and Hydrogen Electrocatalysis	626
<i>Ashton Aleman, Gaurav A. Kamat, Aniket Sandip Mule, Melissa E. Kreider, Michaela Burke Stevens, Thomas F. Jaramillo</i>	
678d Electrochemical Steady State Isotopic Transient Kinetic Analysis (eSSITKA): A New Technique for the Evaluation of Electrocatalytic Materials.....	628
<i>Abigail Circelli, Ezra Clark</i>	
678e Effect of Subsurface Hydrogen and β -PdH _x Phase on the Selective Electrochemical Hydrogenation of Cis,Cis-Muconic Acid.....	629
<i>Deep Patel, Prathamesh Prabhu, Jean-Philippe Tessonnier, Luke Roling</i>	
678f Programmable Catalysis for Steam Reforming of Methane on Ruthenium Catalysts.....	630
<i>Veera Venkata Ramprajwal Vempatti, Shengguang Wang, Lars Grabow</i>	
678g Correlating Experimentally Determined CO Binding Energy with Electrochemical CO Reduction Performance on Cu Surface.....	631
<i>Haocheng Xiong, Bingjun Xu, Qi Lu</i>	
678h Interfacial Electric Field Modulated Catalysis	632
<i>Mingyu Wan, Jun Li, Fanglin Che</i>	

FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE V: CATALYSIS OVER METALS, BIMETALLICS AND SINGLE METAL ATOMS

679b Long-Range Catalytic Effects Uncovered By Atomically Precise Active Site Control in Pd-Zn Intermetallic Catalysts	633
<i>Griffin A. Canning, Haoran He, Angela Ngyuen, Kathryn MacIntosh, Anish Dasgupta, Michael Janik, Robert Rioux</i>	
679c Generalized Trends of Hydride-Mediated C-H Bond Formation on TiO ₂ -Supported Single Atom Catalysts	634
<i>Jeremy Hu, Mikyung Hwang, Michael Janik, Konstantinos Alexopoulos</i>	
679d Probing the Influence of Adsorbate-Adsorbate Interactions on H* and O* Coverage over Pt and Ni Nanoparticles	635
<i>Ayodeji Omoniyi, Isabella Furrick, Alyssa Hensley</i>	
679e Theoretical Assessments of Pd-Pdo Phase Transformation and Its Impacts on H ₂ O ₂ Synthesis and Decomposition Pathways.....	636
<i>Manasi Vyas, Jair Fernando Fajardo Rojas, Diego Gomez Gualdron, Stephanie Kwon</i>	

679f Adhesion Energy Trends for Catalytic Metal Nanoparticles on Carbon and Oxide Supports with Applications in Predicting Performance	638
<i>Nida Janulaitis, Kun Zhao, John Rumpitz, Charles Campbell</i>	
679h Mapping Cooperative Adsorption of Ligands on Metal Nanoparticle Surfaces	639
<i>Rong (rocky) Ye</i>	

HYDROCARBON CONVERSION II: FUNDAMENTALS OF CATALYST DESIGN

682a Tuning the Local Coordination Environment of Ni in Ni/CeO ₂ Catalyst for More Efficient Dry Reforming of Methane	640
<i>Murtadha Almousawi, Shaohua Xie, Fudong Liu</i>	
682b Maximizing Metal Functionality of Ppm Pt in HZSM-5 for Efficient Light Alkanes Dehydroaromatization	642
<i>Yizhi Xiang, Genwei Chen, Hossein Toghiani</i>	
682c Single Ni ²⁺ Active Sites Isolated on Polyoxometalates for Light Olefin Oligomerization	643
<i>Alba Scotto d'Apollonia, Yoonrae Cho, Allen Oliver, Jason Hicks</i>	
682d Fundamental Insights into Non-Oxidative Methane Conversion on Group III-Nitrides	644
<i>Samji Samira, Rebekah Anderson, Phillip Christopher</i>	
682e Tuning External Surface of Mo/H-ZSM-5 Catalysts By Atomic Layer Deposition and Its Impact in Methane Dehydroaromatization	645
<i>Jordy Ramos Yataco, Selim Alayoglu, Justin Notestein</i>	
682h Elucidating the Active Sites and Reaction Location during 1-Butene Isomerization	647
<i>Karoline Hebisch, Pawel A. Chmielniak, Risha Goel, Carsten Sievers</i>	
682g Effects of TiO ₂ Structure on the Methane Partial Oxidation over IrO _x /TiO ₂ Nanomaterials	649
<i>Li-Yin Hsiao, Hanqin Zhao, Helena Hagelin Weaver</i>	

HYDROCARBON CONVERSION III: REACTOR AND PROCESS DESIGN STRATEGIES

683a Enhancing Selectivity, Rate, and Stability in Lscf Membrane/Na ₂ WO ₄ Catalyst Reactors for Oxidative Coupling of Methane: Multi-Functional Layered Hierarchical Systems	650
<i>James Wortman, Rawan Almallahi, Suljo Linic</i>	
683b Rethinking Conventions for Methane Partial Oxidation to a Methyl Ester with Heterogeneous Catalysts	651
<i>Andrea Blankenship, Yinjie Ji, Manoj Ravi, Mark Newton, Jeroen A. van Bokhoven</i>	
683c Tri-Reforming of CH ₄ and CO ₂ to Syn-Gas over Nickel Catalyst Supported on Zirconia Derived Metal Organic Frameworks (MOFs) Catalyst	653
<i>Akansha Pandey, Prakash Biswas</i>	
683d Selective Methanol Oxidation to Formaldehyde in a Chemical Looping System: A Promising Alternative	654
<i>Sonu Kumar, Anuj Joshi, Zhuo Cheng, Melissa Marx, Yehia Khalifa, Amanda Trout, Sudeshna Gun, Zain Mohammad, Liang-Shih Fan</i>	
683e Methane Reforming and Sequential Fischer-Tropsch: A Modeling Study of a Single-Reactor Process	655
<i>Brian Gray, John Kuhn, Babu Joseph</i>	

683f Tuning 1,3-Butadiene Selectivity from Ethanol with Induction Heating	656
<i>Han Wang, John Pham, Nicholas Wang, John O'Donnell-Sloan, Carlos L. Pueyo, Jian-Ping Chen, Erdem Sasmaz</i>	
683g The Role of Gas-Phase Promoters within Propylene Epoxidation By O ₂ over Ag.....	657
<i>Joseph Esposito, Aditya Bhan</i>	
683h Post-Synthetic Approach to Enhance the Catalytic Stability and Regenerability of Mo/ZSM-5 Catalysts for Shale Gas Dehydroaromatization.....	658
<i>Jong Hun Kang, Yangho Jeong, Yong Hyun Lim, Do Heui Kim</i>	

ELECTROCHEMICAL ENGINEERING: REACTOR DESIGN AND REACTION TRANSPORT PROCESSES IN ELECTROCATALYSIS II

671a Hydrogen Peroxide Electrosynthesis in a Strong Acidic Environment Using Cationic Surfactants.....	659
<i>Zachary Adler, Haotian Wang</i>	
671b Engineering Reactors for the Electrochemical Nitrogen Oxidation Reaction Via Advanced Manufacturing	660
<i>Natalie Hwee, Aditya Prajapati, Jennifer Moreno, Jenna Ynzunza, Jonathan Davis, Huiyun Jeong, Sneha Akhade, Jeremy T. Feaster</i>	
671c Electrooxidation of Cyclohexene By Halogen Intermediates in a Liquid Diffusion Electrode Cell.....	661
<i>Adrien Deberghes III, Linsey Seitz</i>	
671d Electrochemical Reduction of CO to Liquid C ²⁺ Products with Enhanced Selectivities at 100 Bars.....	663
<i>Nishithan Balaji Chidambara Kani, Ishita Goyal, Meenesh R Singh</i>	
671e Building the Next Generation of Electrochemical Reactors through Advanced Manufacturing	664
<i>Aditya Prajapati, Natalie Hwee, Jenna Ynzunza, Jonathan Davis, Daniel Corral, Joshua R. DeOtte, Victor Beck, Thomas F. Jaramillo, Sarah Baker, Eric B. Duoss, Sneha Akhade, Jeremy T. Feaster</i>	
671f Selective Electroreduction of CO ₂ to Ethylene Under Controlled Catalyst Regeneration.....	665
<i>Nitin Minocha, Rohan Sartape, Meenesh R Singh</i>	
671g Integrating Direct Air Capture and Ocean Carbon Capture with Photocatalytic CO ₂ Conversion.....	667
<i>Shu Hu</i>	
671h Hydrodynamics Change Tafel Slopes in Electrochemical CO ₂ Reduction on Copper.....	669
<i>Zachary Schiffer, Nicholas Watkins, Yungchieh Lai, Charles B. Musgrave, Harry Atwater, William Goddard III, Theodor Agapie, Jonas C. Peters, John Gregoire</i>	

MICROPOROUS AND MESOPOROUS MATERIALS II: STRUCTURE-PROPERTY RELATIONSHIPS

690a Deconvolution of Solvent Effects on Confined Zeolites: Influences of Partial Solvation and Alkyl Chain Length on Vapor-Phase Epoxidation.....	670
<i>Ohsung Kwon, David Potts, E. Zeynep Ayla, David Flaherty</i>	

690b Second Sphere Coordination Effects in Heterogeneous Redox Catalysis over Highly Uniform Trimetal-Oxo Clusters	671
<i>Jacklyn Hall, Praveen Bollini</i>	
690c Evolution and Distribution of MoO _x Species in Mo-Oxide-Impregnated H-ZSM-5 Catalyst for Methane Dehydroaromatization (MDA)	672
<i>Fateme Molajafari, Emanuele Joy, Sheima Khatib, Joshua Howe</i>	
690e Determination of Catalytic Site Distributions and Contributions for Epoxide Ring Opening in Lewis Acidic Zeolite Sn-Beta.....	673
<i>Leah Ford, Alexander Spanos, Nicholas Brunelli</i>	
690f CO Oxidation over Metal Phthalocyanines Encapsulated in Faujasite Zeolites.....	674
<i>Ethan Iaia, Ganesh Rana, Ademola Soyemi, Tibor Szilvasi, Martin G. Bakker, James W. Harris</i>	
690g Effects of Coordination Environment on the Reactivity, Selectivity, and Stability of Iron Carboxylate MOFs for Peroxide-Mediated Alkene Oxidation	676
<i>Rachel A. Yang, Michele Sarazen</i>	
690h Presence of Multiple Types of Cu Active Sites and Their Connections to Framework Composition and Methane Oxidation Reactivity in Cu-CHA	677
<i>Jose Rebolledo Oyarce, Yujia Wang, Laura Wilcox, Rajamani Gounder, William Schneider</i>	

MICROPOROUS AND MESOPOROUS MATERIALS III: KINETICS AND MECHANISMS

691a Effects of Acid Site Proximity in CHA Zeolites on Monomolecular Propane and n-Butane Activation Kinetics	678
<i>Bereket Bekele, Rajamani Gounder</i>	
691b Structurally Diverse Hierarchical Zeolites for Hydrocarbon Upgrading	679
<i>Michele Sarazen</i>	
691c Unraveling the High NH ₃ Decomposition Activity of Ru-Exchanged 13X Zeolites	680
<i>Sungil Hong, Giannis Mpourmpakis</i>	
691d Using Machine Learning Interatomic Potentials to Understand Water Structure in Zeolites for Sustainable Fuels	681
<i>Mingze Zheng, Brandon Bukowski</i>	
691e Computational Modeling of Bimolecular Hydrocarbon Transformations in Brønsted-Acid Zeolites	682
<i>Shubham Malviya, Peng Bai</i>	
691f A Kinetic, Spectroscopic, and Theoretical Study on Toluene Alkylation with Ethylene on Acidic Mordenite.....	683
<i>Kemakorn Ithisuphalap, Michelle Nolen, Hanna Monroe, Stephanie Kwon</i>	
691g Quantifying the Role of Structure Directing Agents and Framework Al Location on Xylene Isomer Selectivity during Toluene Methylation Reactions.....	684
<i>Hansel Montalvo-Castro, Sopuruchukwu Ezenwa, Huston Locht, Alexander Hoffman, Rajamani Gounder, David Hibbitts</i>	
691h Sustainable Pathways to Acrylic Acid – Conversion of Lactate Feeds over FAU-Based Zeolite Composite Catalysts	685
<i>Benjamin R. Hoekstra, Paul J. Dauenhauer, Christopher P. Nicholas</i>	

CATALYSIS AND REACTION ENGINEERING IN LIQUID AND MULTIPHASE SYSTEMS **II: REACTION MECHANISMS AND REACTOR DESIGN**

559e Optical Sequencing of Single Synthetic Polymers in Liquid.....	687
<i>Rong (rocky) Ye</i>	
559c Integration of Catalytic Membranes and Bio-Hydrogen for Water Detoxification.....	688
<i>Dibakar Bhattacharyya, Rollie Mills, J. Todd Hastings, Michael Detisch, Noah D. Meeks</i>	
559b Mechanistic Insights into the Catalytic Transfer Hydrogenation of Muconic Acid in Solvents.....	689
<i>Haseena K V, M. Ali Haider</i>	
559d Zn ²⁺ -Catalyzed Homolysis of C-Br Bond in α -Bromoethylbenzene: An Efficient Free Radical Generation Mechanism.....	690
<i>Tianyu Deng, Binhang Yan</i>	
559a Computational Study of Reaction Mechanisms in Epoxide Ring-Opening By Aryl Borane Catalysts	691
<i>Guanhua Wang, Hiyab Mekonnen, Carlos Villa, Arjun Raghuraman, Varinia Bernales, Sukaran S. Arora, Saket Sanjay Bhargava, Justin Notestein, Linda J. Broadbelt</i>	
559f Rational Design of Rh/TiO ₂ Catalyst Via Atomic Layer Deposition (ALD) to Improve Hyperpolarization of Allyl Esters from Parahydrogen	692
<i>Hanqin Zhao, Michelle Lapak, Clifford R. Bowers, Helena Hagelin Weaver</i>	
559h Development of a Deep Neural Network for the Prediction of Local Gas Holdup Profiles in Bubble Columns	693
<i>Sebastian Uribe, Ahmed Alalou, Muthanna Al-Dahhan</i>	

REACTION CHEMISTRY AND ENGINEERING II

700b Chemoselective Hydrogenation of Aromatic Carboxylic Acids on TiO ₂ -Supported Single Atom Catalysts	694
<i>Jeremy Hu, Michael Janik, Konstantinos Alexopoulos</i>	
700c Elucidating the Reaction Chemistry of δ -Valerolactone (DVL) Production for Biocompatible, Chemically Recyclable Polyesters.....	695
<i>Raka G. Dastidar, Javier Chavarrio Canas, Zhen Jiang, Manos Mavrikakis, George Huber</i>	
700d Forced Dynamic Operation of Propylene Selective Oxidation to Acrolein.....	696
<i>Mohammad Moniruzzaman, Michael Harold, Lars Grabow</i>	
700e Automated Generation of a Chemical Kinetic Reaction Mechanism for Combustion of N-Hexadecane and Larger Alkanes	698
<i>Venus Amiri, Rubik Asatryan, Mark Swihart</i>	
700f Mechanistic Study of Se-Catalyzed Oxidative Carbonylation of Alcohol for Producing Dialkyl Carbonate	699
<i>Hye Jin Lee, Jayeon Baek, Yong Jin Kim</i>	
700g The Mechanism of Ultrasound-Driven OH-Mediated Aqueous Benzyl Alcohol Oxidation with Analogies to Atmospheric Chemistry.	701
<i>Ari Fischer, Teseer Bahry, Roberto Batista Da Silva Junior, Francois Jerome, James Kwan, Wen Liu, Sabine Valange, Prince N. Amaniampong, Tej Choksi</i>	

INTENSIFIED REACTOR DESIGN AND REACTIVE SEPARATIONS

686a Quaternized Poly(4-vinylpyridine) Catalytic Membranes for Integrated CO ₂ Capture and Conversion.....	703
<i>Casey O'Brien</i>	
686b On the Benefits of Counter-Current Regeneration for a Partial Pressure Swing Adsorptive Reactor (PPSAR) with Application to the Water Gas Shift Reaction	704
<i>Nicholas Margull, Theodore Tsotsis, Vasilios Manousiouthakis</i>	
686e High Pressure Fluidized Bed Reactors	705
<i>Eloy Flores III, Veshal Venkat</i>	
686c Recent Developments in Lithium Silicates for Pre-Combustion CO ₂ Capture	706
<i>Michael Smith, Charles Coe</i>	
686f Building Catalysts, Reactors and Engineers for a Sustainable Future.....	707
<i>Jeremy T. Feaster</i>	

Author Index