

Catalysis and Reaction Engineering Division 2018

Core Programming Area at the 2018 AIChE Annual Meeting

Pittsburgh, Pennsylvania, USA
28 October - 2 November 2018

ISBN: 978-1-5108-7616-3

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© (2018) by AIChE
All rights reserved.

Printed by Curran Associates, Inc. (2019)

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

(14a) Low Temperature NO and Hydrocarbon Trapping over Pd-Exchanged Zeolite Passive NO_x Adsorbers	1
<i>Sam Malamis, Michael Harold</i>	
(14b) Ion-Exchanged Zeolites for Hydrocarbon Traps and Passive NO_x Adsorption Applications	2
<i>Jungkuk Lee, Vivek Vattipalli, Wei Fan, Eleni A. Kyriakidou</i>	
(14c) Excellent Hydrothermal Stability of Composite Catalyst Based on Two Cu-CHA Type Molecular Sieves	3
<i>Yuhan Ma, Yongdan Li</i>	
(14d) Effects of Surface Species and Dispersion of CeO₂ Supported Transition Metal Oxide Catalysts for NO Reduction By CO Reaction	4
<i>Shuhao Zhang, Taejin Kim</i>	
(14e) Fast Lean-Rich Cycling for Enhanced NO_x Conversion on Pt/CeO₂/Al₂O₃	5
<i>Zhiyu Zhou, Michael Harold, Dan Luss</i>	
(14f) Degrading Organic Compounds in Simulated Produced Water By Creating Hydroxyl Radicals Catalytically	7
<i>Yiyuan Yin, Kimberly N. Heck, Camilah Powell, Christian L. Coonrod, Sujin Guo, Michael S. Wong</i>	
(14g) Swellable Organically Modified Silica (SOMS): A Novel Support for Pd Catalyzed Hydrodechlorination of Trichloroethylene in Aqueous Phase	8
<i>Gokhan Celik, Saurabh Ailawar, Seval Gunduz, Jeffrey T. Miller, Franklin (Feng) Tao, Paul Edmiston, Umit S. Ozkan</i>	
(14h) Treatment of OIL Produced Water Using Advanced Oxidative Processes: Heterogeneous-Photocatalysis and Photo-Fenton	9
<i>Priscila C. Silva, Nathalia P. Ferraz, Elen A. Perpetuo, Yvan J. O. Asencios</i>	
(14i) Electrochemical Anthraquinone Process Enabled By Phase Transfer Catalysis	12
<i>Sahag Voskian, Alexander T. Murray, Yogesh Surendranath, T. Alan Hatton</i>	
(21a) Anatase Nanoparticles from Low Pressure Flame Synthesis for Enhanced Photocatalytic Activity	13
<i>Ashley M. Pennington, Fuat E. Celik, Stephen D. Tse</i>	
(21b) Application of Ti-Doped MoO₂ microspheres Prepared By Spray Pyrolysis to Partial Oxidation of N-Dodecane	14
<i>Qusay Bkour, M. Grant Norton, Su Ha</i>	
(21c) Fundamental Mechanistic Studies of Formic Acid Decomposition on Pd Catalysts	15
<i>Saurabh Bhandari, Srinivas Rangarajan, Sha Li, Suyash Singh, Christos Maravelias, James Dumesic, Manos Mavrikakis</i>	
(21d) The Effect of Nickel and Magnesium Loadings on the Activity, Selectivity and Stability for Catalytic Dry Reforming of Biogas Using Pt/Cerium-Zirconium Oxide Catalyst	16
<i>Yetunde O. Sokefun, Babu Joseph, John N. Kuhn</i>	
(21e) Intrinsic Kinetics of Steam Methane Reforming on a Thin, Nanostructured and Adherent Ni Coating	17
<i>Florent Minette, Michael Lugo, Dean Modroukas, Andrew W. Davis, Rajinder Gill, Marco J. Castaldi, Juray De Wilde</i>	
(21f) Development of Metal-Rich Two-Dimensional Catalysts for Highly Efficient Hydrogen Evolution Reaction	18
<i>Alireza Kondori, Chris Coble, Mohammad Asadi</i>	
(21g) Comparison of the Direct and Bifunctional Mechanisms through Steady-State Microkinetic Modeling for Hydrogen Electrocatalysis in Alkaline Media	19
<i>Luis Rebolgar, Maureen H. Tang</i>	
(31a) Methane (sI) Hydrate Crystallization and Dissociation in a Thermoelectrically-Cooled Microreactor	20
<i>Weiqi Chen, Bruno Pinho, Ryan L. Hartman</i>	
(31b) C-H Activation By Ozone in Liquid CO₂	21
<i>Xuhui Chen, Derek Rice, Andrew Danby, Michael D. Lundin, Timothy Jackson, Bala Subramaniam</i>	
(31c) pH Sensitive Colloidal Gold Nanoparticle Catalysts for Enhanced Recovery and Reuse	22
<i>Saptarshi Chakraborty, Christopher L. Kitchens</i>	
(31d) CO₂ Conversion Via RWGS-CL over La-Perovskite Oxide with Three Metals (Co, Fe, and Mn) in the B-Site	23
<i>Adela E. Ramos, Debitanu Maiti, Yolanda Daza, J. N. Kuhn, Venkat R. Bhethanabotla</i>	
(31f) High Performance Non-Mercury Catalysts for VCM Production: From Theoretical Study to Industrialization	24
<i>Hao Xu, Guohua Luo</i>	
(31g) Chloroplast-Inspired Artificial Photosynthetic Capsules for Efficient and Sustainable Enzymatic Hydrogenation	29
<i>Jiafu Shi</i>	
(41b) Enhanced CO₂ Electroreduction in Selectivity Tuned By Anion Modification of the Ionic Liquids	30
<i>Jianpeng Feng, Shaojuan Zeng, Suojiang Zhang, Xiangping Zhang</i>	
(41c) Understanding the Role of Ionic Liquids in the Enzyme Catalyzed Breakdown of Cellulose Using Molecular Dynamics Simulations	31
<i>Sarah Alamdari, Jim Pfaendmer</i>	
(41d) Novel Ionic Liquids Preparation and Application in Gas Separation Process	32
<i>Haifeng Dong, Shaojuan Zeng, Xiangping Zhang, Suojiang Zhang</i>	
(41e) Isobutane Alkylation with C4 Olefin Catalyzed By Combination of so₃h-Functionalized Ionic Liquids and Sulfuric Acid	33
<i>Weizhong Zheng, Piao Cao, Weizhen Sun, Ling Zhao</i>	

(41f) Superoxide-Derived CO₂ Reduction at Low over-Potentials and Ultra-Fast: A General Approach in Ionic Liquids	34
<i>Zhe Wang</i>	
(41g) Biocatalysis in Anhydrous Ionic Liquids	35
<i>Jason P. Hallett, Alex Brogan</i>	
(46b) Investigation of Bimetallic Mn-Fe Oxygen Carriers for Coal in Situ Gasification Chemical-Looping Combustion (iG-CLC)	36
<i>Ping Wang, Nicholas C. Means, Bret H. Howard, Dushyant Shekhawat</i>	
(46c) An Examination of HONO and HNO₂ in Low-Temperature Combustion	37
<i>Mark Fuller, C. Franklin Goldsmith</i>	
(46d) Pyrolytic Remediation of Oil-Contaminated Soils: Reaction Mechanisms and Treated Soil Fertility	38
<i>Julia E. Vidonish, Pedro J. J. Alvarez, Kyriacos Zygourakis</i>	
(46e) Effect of Temperature and Transport on the Yield and Composition of Pyrolysis-Derived Bio-Oil	39
<i>Khurshheed B. Ansari, Jyotsna S. Arora, Jia Wei Chew, Paul Dauenhauer, Samir H. Mushrif</i>	
(46f) Comparison between Catalytic Fast Pyrolysis and Catalytic Fast Hydropyrolysis of Arundo Donax in a Fluidized Bed Reactor	40
<i>Devin Chandler, Fernando Resende</i>	
(46g) A Framework for Chemical Kinetics Extraction Based on Reactive Molecular Dynamics	41
<i>Srujan Rakkam, Kiran Sasikumar, Raghavan Ranganathan, Peter Cross, Richard Burnes</i>	
(47a) Magnetic Imaging to Model Olefin Product Yields from High Severity Naphtha Cracking	42
<i>Preetinder S. Virk</i>	
(47b) Reaction Coupling of Propane Dehydrogenation and Nitrobenzene Hydrogenation	43
<i>Peng Yu, Hsi-Wu Wong</i>	
(47c) Tuning Solid Catalysts to Control Regioselectivity in Cross-Aldol Condensations with Unsymmetrical Ketones	44
<i>Koushik Ponnuru, Jinesh Manayil, Hong Je Cho, Wei Fan, Karen Wilson, Friederike C. Jentoft</i>	
(47e) Importance of Explicit Solvent Molecule Inclusion in Predicting Electrolyte Reduction Kinetics in Lithium Ion Batteries	45
<i>Mathew J. Boyer, Gyeong S. Hwang</i>	
(47f) Software Tools for Developing Molecular-Level Kinetic Models of Large, Complex Chemical Systems	46
<i>Pratyush Agarwal, Juan Lucio-Vega, Michael T. Klein</i>	
(73a) Assessing Discrepancies in Kinetic Parameters and Improving Combustion Models through Metaheuristic Optimization	47
<i>Nathan Harms, Sai Krishna Sirumalla, Richard H. West</i>	
(73b) Automated Discovery of Reaction Pathways for the Combustion of Alternative Fuel Candidates	48
<i>Ahmed E. Ismail</i>	
(73c) A Computational Investigation into the Kinetics of NO + CH₂CCH and Its Effect on NO Reduction	49
<i>Aaron Danilack, C. Franklin Goldsmith</i>	
(73d) Diluent Effect on NO_x Formation in Pressurized Combustion of Syngas/Air	50
<i>Nazli Asgari, Ryan Cichowicz, Bihter Padak</i>	
(73e) Ash Partitioning and Ultrafine Aerosol Formation Mechanism for Air and Oxy-Combustion of Coal, Biomass and Blends	51
<i>Yueming Wang, Xiaolong Li, Jost O. L. Wendt</i>	
(73f) Effect of SO₂ on CuMn₂O₄ Oxygen Carrier's Reactivity for Chemical Looping with Oxygen Uncoupling (CLOU)	52
<i>Turna Barua, Sam Horlick, Bihter Padak</i>	
(73g) Simultaneous Removal of Hg(0) and NO over Modified SCR Catalyst	53
<i>Can Li, Zhouyang Liu, Vishnu Sriram, Joo-Youp Lee</i>	
(79a) Experimental and Theoretical Studies of the Electrochemical Reduction of CO₂ on Cu	54
<i>Alexis T. Bell</i>	
(79b) Highly Efficient CO Electroreduction Catalyst Based on Polycrystalline Cu Particles	55
<i>Jing Li, Qi Lu</i>	
(79c) Operando Spectroscopic Investigations of Oxide Derived Metal Catalysts for CO₂ and CO Reduction	56
<i>Arnav Malkani, Marco Dunwell, Bingjun Xu</i>	
(79d) Molecular-Level Insights into Electrocatalytic Carbon Dioxide Reduction at Cobalt Macrocycles	57
<i>Karthish Manthiram</i>	
(79e) Mass Transfer Effects in CO₂ Reduction Electrocatalysis	58
<i>Chao Wang</i>	
(79f) Single Atom Catalysts for Electrochemical Reduction of CO₂	59
<i>Aditya Prajapati, Songwei Che, Vikas Berry, Meenesh R. Singh</i>	
(79g) Photoelectrochemical CO₂ Reduction at Plasmonic Nanostructured Silver Electrodes	60
<i>Elizabeth R. Corson, Erin B. Creel, Youngsang Kim, Matthew J. Liu, Davis D. Perez, Jeffrey J. Urban, Robert Kostecki, Bryan D. McCloskey</i>	
(90a) Maximizing Efficiencies of Photocatalytic Water Splitting By Engineering Interfaces in Multi-Component Photocatalysts	61
<i>Suljo Linic</i>	
(90b) Recent Advances in Zeolite-Based Technologies	62
<i>Javier Guzman</i>	
(90c) Direct Synthesis of H₂O₂ from H₂/O₂ Mixtures and Its Decomposition over Intermetallic Pd-Zn Catalysts	63
<i>Tianze Xie, Anish Dasgupta, Robert Rioux</i>	

(90d) Oxygen Electrocatalysis Using Layered Mixed Metal Oxides	64
<i>Eranda Nikolla</i>	
(90e) Improved Carbon Coatings for Nitrogen Production and Upgrading Pyrolysis Oils	65
<i>Charles Coe</i>	
(90f) Hybrid Materials for Catalysis and Separations	66
<i>Daniel F. Shantz</i>	
(90g) Structural and Dynamic Characteristics of Supported Metal Catalysts at the Atomic Scale	67
<i>Phillip Christopher</i>	
(90h) Carbide-Based Electrocatalysts in Alkaline Electrolyte	68
<i>Jingguang G. Chen</i>	
(101a) Earth Abundant Perovskite Oxides for Low Temperature CO₂ Conversion	69
<i>Debtanu Maiti, Bryan J. Hare, Adela E. Ramos, Yolanda A. Daza, John N. Kuhn, Venkat R. Bhethanabotla</i>	
(101b) Rationalizing the Reactivity of Bimetallic Molecular Catalysts for CO₂ Hydrogenation	70
<i>Jingyun Ye, Ryan C. Cammarota, Jing Xie, Matthew Vollmer, Laura Gagliardi, Connie C. Lu, Christopher Cramer, Donald G. Truhlar</i>	
(101c) Physical Descriptors That Control Metal-Support Interactions Identified with DFT and Statistical Learning	71
<i>Thomas P. Senfile</i>	
(101d) Examining Acid Formation during the Selective Dehydration of Fructose to 5-Hydroxymethylfurfural in DMSO and Water	72
<i>Mariah Whitaker, Aamena Parulkar, Rutuja Joshi, Nicholas Brunelli</i>	
(101e) Does Hydrophobic Modification of Solid Acid Catalysts Promote Water Tolerance during Condensed Phase Catalytic Reactions of Oxygenates?	73
<i>William Elliott, Yanyu Mu, Isabel Burgos, Joann Sutyak, Robert M. Rioux</i>	
(101f) Designing Immobilized Tertiary Amine Catalysts for Selective Isomerization of Glucose to Fructose	74
<i>Nitish Deshpande, Lagnajit Pattanaik, Mariah Whitaker, Chi-Ta Yang, Li-Chiang Lin, Nicholas Brunelli</i>	
(101g) Supported Gold Clusters with Modulated Environment for Catalysis	75
<i>Nidhi Kapil, Michael M. Nigra, Marc-Olivier Coppens</i>	
(102a) In-Flow Production of Levoglucosenone from the Catalytic Dehydration of Cellulose Using Homogeneous Bronsted Acid Catalysts in γ-Valerolactone	76
<i>Alexa M. Gonzalez-Rosario, Oscar Oyola-Rivera, Nelson Cardona-Martinez</i>	
(102b) Cyclooctene Cooxidation-Facilitated Co-ZSM-5-Catalyzed Selective Oxidation of Ethylbenzene with Molecular O₂	77
<i>Anyang Peng, Matthew Ross, Linping Qian, Maxfair C. Kung, Brian Hoffman, Harold H. Kung</i>	
(102c) Dirhodium Immobilized Hollow Fiber Flow Reactor for Scalable and Sustainable C-H Functionalization in Continuous Flow	78
<i>Chun-Jae Yoo, Daniel Rackl, Wenbin Liu, Caroline Hoyt, Brian R. Pimentel, Ryan Lively, Huw M. L. Davies, Christopher W. Jones</i>	
(102d) Catalytic Dehydration of Levoglucosan and Cellulose to Levoglucosenone Using Bronsted Solid Acid Catalysts in Tetrahydrofuran	79
<i>Oscar Oyola-Rivera, Jiayue He, George W. Huber, James A. Dumesic, Nelson Cardona-Martinez</i>	
(102e) Composite Hollow Fiber Microfluidic Catalytic Reactors for Direct Conversion of Glucose to 5-HMF	80
<i>Yingxin He, Fateme Rezaei, Ali Rownaghi</i>	
(102f) Water Soluble Palladium-β-Cyclodextrin Complex and Its Catalytic Performance for a Suzuki-Miyaura Cross-Coupling in Flow	81
<i>Yukun Liu, Ryan L. Hartman</i>	
(102g) Regioselective Epoxide Ring Opening with Alcohols Using Heterogeneous Lewis Acid Catalysts	82
<i>Nitish Deshpande, Nicholas Brunelli, Aamena Parulkar, Rutuja Joshi, Alexander Spanos</i>	
(120b) 2018 Outlook for Energy: A View to 2040	83
<i>Theodore J. Wojnar Jr.</i>	
(120c) Energy Decarbonisation Scenarios	84
<i>Kamel Ben Naceur</i>	
(120a) Fundamental Research Needs to Advance Energy Technologies	85
<i>Bruce Garrett</i>	
(145a) Electrochemical CO₂ Conversion to Valuable Chemicals	86
<i>Feng Jiao</i>	
(83h) Development of Devices and Selective Catalysts for the Solar-Driven Reduction of CO₂ to fuels	87
<i>Marcel Schreier, Michael Gratzel, Yogesh Surendranath</i>	
(145c) Bimetallic Nanoporous Pd Alloys as CO Tolerant Electrocatalysts for the Electrohydrogenation of CO₂ to Formate	88
<i>Swarnendu Chatterjee, Yawei Li, Joshua Snyder</i>	
(145d) Electrochemical Promotion of Catalysis: Non-Faradaic Effects of Applied Potential on CO₂ Hydrogenation and Ethylene Oxidation Reactions	89
<i>Mark Sullivan, Dimitris Zagoraios, Constantinos Vayenas, Yuriy Roman-Leshkov</i>	
(145e) Nano- to Macro Scale Morphological Impacts on CO₂ Electroreduction Product Selectivity over Cu Catalysts	90
<i>Samaneh Sharifi Golru, Alexandros N. Karaiskakis, Elizabeth J. Biddinger</i>	
(145f) Insights into the Electrocatalytic Conversion of CO₂ into CO, Ethylene, and Ethanol in Alkaline Media	91
<i>Paul J. A. Kenis, Andrew A. Gewirth</i>	
(145g) Insights on the Electrochemical Reduction of Carbon Dioxide Using Solid Oxide Electrolysis Cells	92
<i>Juliana S. A. Carneiro, Xiang-Kui Gu, Eranda Nikolla</i>	

(158a) Catalytic C-C Bond Forming Reactions for the Transformation of Biomass to Commodity Chemicals	93
<i>Raul F. Lobo</i>	
(158b) Evidence for Tunable Electronic Metal-Support Interactions in Carbon-Supported Palladium Catalysts	94
<i>Radhika Rao, Raoul Blume, Kathleen Dreyer, Thomas W. Hansen, David Hibbitts, Robert Schlogl, Jean-Philippe Tessonnier</i>	
(158c) Fabrication of Nano-Structured Catalyst Supports By ALD	95
<i>Raymond J. Gorte</i>	
(158d) Template-Mediated Tunability of Pores, Polymorphism, and Function in Nanostructured Materials	96
<i>Mark A. Snyder</i>	
(158e) Unconventional Pathways for Unconventional Feedstock: The Importance of Simultaneous Optimization of Catalytically Active Sites and Their Environment	97
<i>Lars C. Grabow</i>	
(158f) Leveraging DFT with Machine Learning: Applications in Catalysis	98
<i>John R. Kitchin</i>	
(158g) Exploiting Mesoporosity for the Design of Novel Materials	99
<i>Jeffrey D. Rimer</i>	
(158h) Lithium Silicates for High Temperature CO₂ Capture	100
<i>Michael A. Smith</i>	
(160a) Sulfur Poisoning of SCR Catalysts	101
<i>Yasser Jangjou, William S. Epling</i>	
(160b) Overlayer Catalysts: Convincing Ourselves That the Observed Change Is Real	102
<i>Joseph H. Holles</i>	
(160c) Generating Novel Compounds Through Bioprivileged Molecules	103
<i>Brent H. Shanks</i>	
(160d) Interfacial Perimeter Sites in Au-TiO₂ Systems	104
<i>Alex Prokofjevs, Mayfair C. Kung, Harold H. Kung</i>	
(160e) Catalysis Researchers Caused Climate Change: What Can We Do to Reverse It?	105
<i>Christopher W. Jones</i>	
(160f) Insights into Catalytic Oxidation and Reduction Reactions at Metal/Solution Interfaces	106
<i>Matthew Neurock, Ashwin Chemburkar</i>	
(169a) A Density Functional Theory Approach to Electrocatalytic Reaction Barriers	107
<i>Michael J. Janik</i>	
(169b) The Influence of Local Environment on Theoretical Calculations of Adsorption and Reaction for Catalyzed Reactions	108
<i>Alexis T. Bell</i>	
(169c) Tackling the Inverse Design Problem in Quantum Chemistry	109
<i>Daniel S. Lambrecht</i>	
(169d) Computational Alchemy to Drive Searches for Catalysts through Materials Space	110
<i>Charles Griego, Karthikeyan Saravanan, John A. Keith</i>	
(169e) Synergistic Application of XPS and DFT to Investigate Metal Oxide Surface Catalysis	111
<i>Quang Thang Trinh, Kartavya Bhola, Prince N. Amaniampong, Francois Jerome, Samir H. Mushrif</i>	
(169f) Maximal Predictability Approach for Identifying the Right Descriptors for Electrocatalytic Reactions	112
<i>Vaidish Sunaria, Dilip Krishnamurthy, Venkatasubramanian Viswanathan</i>	
(169g) Understanding Structure-Property Relationships in Catalysts By Using Cluster Expansions	113
<i>Chenyang Li, Tim Mueller</i>	
(172a) Statistically Guided Synthesis of MoV-Based Mixed Oxide Catalysts for Ethane Partial Oxidation	114
<i>Juan Jimenez, Kathleen Mingle, Cun Wen, Jochen Lauterbach</i>	
(172b) Periodic Trends in the Morphology, Charge Distribution, and Energetics of Oxygen Vacancies on Doped MoO₃ (010)	115
<i>Tej S. Choksi, Jeffrey Greeley</i>	
(172c) DFT Study on the Catalytic Activity of Oxo-Centered Trimetallic MOF Building Units for Ethane Oxidation to Ethanol	116
<i>Melissa Barona, Sol Ahn, Omar K. Farha, Randall Q. Snurr</i>	
(172d) Highly Efficient Single Pt (Au) Atom Catalysts for Preferential Oxidation of CO (PROX)	117
<i>Sufeng Cao, Maria Flytzani-Stephanopoulos, Jilei Liu</i>	
(172f) Design of Ni-Based Intermetallic Compounds to Promote C-H Bond Cleavage and Control C-C/C=C Bond Activation in the Dehydrogenation of Light Hydrocarbons	118
<i>Yang He, Yuanjun Song, Siris Laursen</i>	
(172g) Studying Sub Nano-Meter Ensemble Effects on Selective Hydrogenation Utilizing the \hat{F}^3-Brass Phase Crystal Structure	119
<i>Anish Dasgupta, Haoran He, Randall Meyer, Michael Janik, Robert Rioux</i>	
(173a) Solvent Reaction Coordinate for an S_N2 Reaction	120
<i>Christian Leitold, Christopher J. Mundy, Marcel D. Baer, Gregory K. Schenter, Baron Peters</i>	
(173b) Importance of Simultaneous Reduction of Gas and Surface Mechanisms in Capturing Dominant Kinetic Features	121
<i>Devi Veerappan, Karthik Ramanathan, Niket S. Kaisare</i>	
(173c) A Kinetic Study of the Ethylene Oligomerization over a Nibea Catalyst	122
<i>Gabriel Seufitelli, Fernando Resende</i>	
(173d) Evaluation of the Thermal Decomposition Products of 2-Nitrotoluene	123
<i>Wen Zhu, Chad Mashuga</i>	

(173e) Modeling of Fast Cycling NO_x Storage and Reduction - Effect of Reductants, Thermal Effect, and HC-Intermediate Mechanism	124
<i>Allen Wei-Lun Ting, Michael Harold, Vemuri Balakotaiah</i>	
(173f) Study on the Competitiveness of Homogeneous Molecular Catalysis for the Continuous Valorization of CO₂ in Organic Solvents	126
<i>Johann-Kilian Schnoor, Marcel A. Liauw</i>	
(173g) Investigating the Effect of Acids and Halides on Direct Synthesis of Hydrogen Peroxide	127
<i>Pranjali Priyadarshini, David Flaherty</i>	
(206a) Experimental Study and Modelling of Kinetic Transitions upon Processing of Dimethyl Ether and Methanol to Gasoline (DMTG) at Fluctuating Workloads	128
<i>Johannes Kunz, Bettina Kraushaar-Czarnetzki</i>	
(206b) Conversion of Ethanol to Distillate Fuels through Guerbet Condensation	131
<i>Nathaniel Eagan, Ashley Wittrig, J. Scott Buchanan, James A. Dumesic, George W. Huber</i>	
(206c) Advanced Reactor Design for CO₂-Methanation	132
<i>Gunnar Ganzer, Christian Schuhbauer, Andreas Heinrich, Rolf Bank</i>	
(206e) Highly Active and Selective Bifunctional Catalyst for One-Step DME Synthesis By CO₂ Hydrogenation	133
<i>Shoujie Ren, Weston R. Shoemaker, Xiaofeng Wang, Zeyu Shang, Naomi Klinghoffer, Shiguang Li, Miao Yu, Xinhua Liang</i>	
(206f) Cobalt Nanoparticles Supported on Graphene for Fischer-Tropsch Synthesis	134
<i>Tamara R Mignoli, Thiago L. R. Hewer, Martin Schmal, Rita M. B. Alves</i>	
(206g) Selective Hydrogenation of 5-Hydroxymethylfurfural to 2,5-Dihydroxymethylfuran Using Octahedral Molecular Sieve Support As Catalyst	138
<i>Jennifer Dicks, Kathryn Ralphs, Manish Tiwari, Laura Marti, Vivek Ranade, Haresh Manyar</i>	
(217a) Integrating Non-Precious Metal H₂ Evolution Catalysts into Water Electrolyzers and Photoelectrochemical Water-Splitting Devices	140
<i>Thomas F. Jaramillo</i>	
(217b) When Electrocatalysis Matters and When It Does Not: Unexpected Observations in Water Electrolysis and Flow Battery Energy Storage	141
<i>James R. McKone</i>	
(217c) Understanding the Role of Adsorbed Hydroxide in Reversible Hydrogen Reactions	142
<i>Saad Intikhab, Joshua Snyder, Maureen H. Tang</i>	
(217d) Electrocatalysis at Buried Interfaces	143
<i>Daniel Esposito</i>	
(217e) Density-Functional-Theory Studies of Face-Centered-Cubic Tungsten Carbide and Pt Core-Shell Nanoparticles Catalysts for the Hydrogen Evolution Reaction	144
<i>Akash Jain, Ashwin Ramasubramaniam</i>	
(217f) Kinetic Investigation of Nickel-Iron Layered Double Hydroxide for Hydrogen Evolution in an Alkaline Electrolyte	145
<i>Aisha Alobaid, Chunsheng Wang, Raymond A. Adomaitis</i>	
(217g) BiVO₄/WO₃ Photoanodes for Chloride Oxidation with Simultaneous H₂ Production	146
<i>Alan Rassoolkhani, Wei Cheng, Austin McKee, Jonathan Koonce, Abdulsattar Alsaedi, Syed Mubeen</i>	
(217h) On the Combustion Synthesis and Characterization of Ga_xZn_{1-x}O_yN_{1-y} for Water Splitting Applications	147
<i>Austin Kennedy, Ben Meekins</i>	
(228a) The Drive for Advantaged on-Purpose Propylene	148
<i>Billy B Bardin, Matt Pretz, Lin Luo</i>	
(228b) Solvent Effects in Acid-Catalyzed Reactions of Biomass-Derived Oxygenates	149
<i>James Dumesic, Max A. Mellmer, Chotitath Sanpitakseree, Benginur Demir, Peng Bai, Kaiwen Ma, Theodore Walker, Alex Chew, Huixiang Li, Z. Conrad Zhang, George W. Huber, Reid C. Van Lehn, Matthew Neurock</i>	
(228c) Synthesis of Chiral Molecular Sieves: A 30 Year Journey	150
<i>Mark E. Davis</i>	
(228d) Atom Trapping: A Novel Approach to Generate Thermally Stable and Regenerable Single Atom Catalysts	151
<i>Abhaya K. Datye, Andrew T. Delariva, Xavier Isidro Pereira Hernandez, Haifeng Xiong, Deepak Kunwar, Christopher Ryan Riley, Eric J. Peterson, Yong Wang</i>	
(228e) Spectroscopic and Transient Kinetic Analyses of Metal Catalysts for the Conversion of Oxygenates	152
<i>Robert J. Davis</i>	
(234a) Modeling Heterogeneous Electrocatalysis on Realistic Surfaces from First-Principles, Thermodynamics, and Machine Learning	153
<i>Andrew M. Rappe</i>	
(234b) Uncovering Reaction Maps to Promote Active Catalysis	154
<i>Paul M. Zimmerman</i>	
(234c) Liquid Phase Modeling in Heterogeneous Catalysis	155
<i>Mohammad Saleheen, Andreas Heyden</i>	
(234d) Improving the Initial Guess for a Nudged Elastic Band Calculation By Incorporating Chemical Intuition	156
<i>Kyle Groden, Jean-Sabin McEwen</i>	
(234e) Improving the Efficiency of Kinetic Monte Carlo Simulations for Catalysis with a Parallel Caching Algorithm	157
<i>Michail Stamatakis</i>	
(234f) Machine Learning Molecular Dynamics for Understanding Nonadiabatic Surface Reactions	158
<i>Jiamin Wang, Hongliang Xin</i>	
(234g) Mapping the Degree of Rate Control Using Automated Construction of Microkinetic Models with Rmg-Cat	159
<i>Emily Mazeau, David Farina Jr., Richard H. West, Katrin Blondal, C. Franklin Goldsmith</i>	

(240a) Elucidating Mechanisms of Plasmon Decay in Multimetallic Nanostructures for the Rational Design of Plasmonic Photocatalysts	160
<i>Steven Chavez, Umar Aslam, Suljo Linic</i>	
(240b) Computational Investigation of Transition Metal Alloying Effects on the Structure and Enhanced Stability of Pt-Ni Nanoparticles	161
<i>Liang Cao, Tim Mueller</i>	
(240c) Design of Non-Stoichiometric Mixed Metal Oxides As Electrocatalysts for Oxygen Reduction	162
<i>Xiang-Kui Gu, John Carl A. Camayang, Samji Samira, Ayad Nacy, Eranda Nikolla</i>	
(240d) Oxide Heterostructure Systems for Oxygen Evolution Reaction - Activation of SrTiO₃ with Subsurface SrRuO₃	163
<i>Aleksandra Vojvodic</i>	
(240e) Overcoming Site Heterogeneity in Search of Metal Nanocatalysts for Oxygen Reduction	164
<i>Siwen Wang, Noushin Omidvar, Emily Marx, Hongliang Xin</i>	
(240f) Active Learning Across Intermetallics Guides Discovery of Electrocatalysts for Carbon Dioxide Reduction and Hydrogen Evolution	165
<i>Kevin Tran, Zachary Ulissi</i>	
(240g) Design of Optimal Metallic Surface Reconstructions for Heterogeneous Catalysis	166
<i>Christopher L. Hanselman, Wen Zhong, Kevin Tran, Zachary Ulissi, Chrysanthos E. Goumaris</i>	
(241a) Continuous Hydrogen Generation for PEM Fuel Cell Vehicles Using Catalytic Decomposition of Hydrous Hydrazine: Experiments and Model	167
<i>Wooram Kang, Arvind Varma</i>	
(241b) Initial Rate Kinetics of Pyrene Polymerization Catalyzed with AlCl₃	168
<i>William Lamie, Mark C. Thies, David A. Bruce</i>	
(241c) Unravelling the Catalytic Effect of Naturally Occurring Inorganics on Biomass Pyrolysis Chemistry: A Combined Experimental and DFT Study	169
<i>Jyotsna S. Arora, Khursheed B. Ansari, Paul Dauenhauer, Samir H. Mushrif</i>	
(241d) Effects of Morphology and Dopants on the CO₂ Capacity of Nanofibrous Calcium-Oxide Based Materials for Sorption-Enhanced Steam Methane Reforming	170
<i>Dante Simonetti, Luke Minardi, Faisal H. Alshafei, Zubin Mishra</i>	
(241e) A Strategy for Developing Structure-Based Kinetic Model for Hydrodesulfurization Reactor Under Petroleomics Concept	171
<i>Thuy T. H. Nguyen, Sho Kataoka, Yuki Takahashi, Koji Tsuji, Ryuzo Tanaka</i>	
(241f) Estimating Kinetic Parameters from Batch Data: Breaking Correlations Using Mixed-Effects Models	172
<i>Daniel W. Trahan, Fabio D'Ottaviano, Michael Ignatowich, Daniel A. Hickman</i>	
(254a) Machine Learning Approaches for Enzyme Engineering	173
<i>Sanjan T. P. Gupta, Evan Glasgow, Brian G. Fox, Parmeswaran Ramanathan, Jennifer L. Reed</i>	
(254b) Simulating the Mechanistic Pathway of Transglycosylation Via a Mutant Glycoside Hydrolase	174
<i>Tucker Burgin, Heather Mayes</i>	
(254c) Engineering a Multifunctional Family 5 Glycosyl Hydrolase into a Transglycosidase	175
<i>Chandrakanth Bandi, Antonio Goncalves, Shishir Chundawat</i>	
(254d) Computational Insights into the Catalytic Function of Processive Cellulases	176
<i>Brandon C. Knott, Joshua Vermaas, Jerry Stahlberg, Gregg T. Beckham, Michael F. Crowley</i>	
(254e) Enhanced Lipase-Catalyzed Hydrolysis and Modification of Fats and Oils	177
<i>Akash Anand</i>	
(254f) Activity Improvement of D-Psicose-3-Epimerase from Agrobacterium tumefaciens CGMCC 1.1488 By Site-Directed Mutagenesis	184
<i>Xiaoyan Chen, Shijie Liu, Zhenhong Yuan, Jingliang Xu</i>	
(269a) Modelling of the Dynamic Behavior of Catalyst Materials in Reacting Conditions: An Application to the Catalytic Partial Oxidation of Methane on Rhodium	185
<i>Raffaele Cheula, Aloysius Soon, Matteo Maestri</i>	
(269b) Effects of Dopant Loading and CO Adsorption on the Structural Stability of Highly Dilute Alloys	188
<i>Konstantinos Papanikolaou, Matthew Darby, Michail Stamatakis</i>	
(269c) Unravelling Hydrogenation Barriers for CO₂ Reduction on Nitrogen Doped Zigzag Edges of Graphene	189
<i>Yasemin Basdogan, John A. Keith</i>	
(269d) Overcoming Ammonia Synthesis Scaling Relations with Plasma-Enabled Catalysis	190
<i>Prateek Mehta, Patrick Barboun, Francisco Herrera, David Go, Jason C. Hicks, William F. Schneider</i>	
(269e) How Do DFT+U and Hybrids Alter Widely Applied Linear Scaling Relations in Heterogeneous Catalysis?	191
<i>Qing Zhao, Heather J. Kulik</i>	
(269f) Grand Canonical DFT Investigation of CO₂ Electroreduction on Noble and Transition Metal Surfaces	192
<i>Dominic Alfonso, De Nyago Tafen, Douglas R. Kauffman</i>	
(269g) Determination of H₂O-Solvated Cationic Fe(III) Coordination Geometry in Fe-SSZ-13 Using Wavefunction Coupled-Cluster Parameterized Hybrid Density Functional Theory	193
<i>Sichi Li, William F. Schneider</i>	
(269h) Coverage Dependent Adsorption of Phenol on Pt (111): Estimating the Lateral Interactions Exhibited By Bio-Oil Model Compounds Under Hydrodeoxygenation Reaction Conditions	194
<i>Neeru Chaudhary, Abyssa Hensley, Yong Wang, Jean-Sabin McEwen</i>	
(280a) Stability of Platinum in the Electrochemical Environment: Reconstruction, Roughening, and the Third Peak	196
<i>Ian T. McCrum, Michael A. Hickner, Michael J. Janik, Marc T. M. Koper</i>	

(280b) Sustainable Synthesis of Electrocatalytic Bismuth-Based Core-Shell and De-Alloyed Nanoparticles	197
<i>Anastasios Angelopoulos, Kevin Tonnis, Junchuan Fang</i>	
(280c) Atomically Dispersed and Nitrogen Coordinated Metal Site Catalysts for Oxygen Reduction in Acids	198
<i>Gang Wu</i>	
(280d) Oxygen Reduction Reaction over a Novel 3D Pt-Supported Vertically Aligned Carbon Nanofiber	199
<i>Jiayi Xu, Ayyappan Elangovan, Jun Li, Bin Liu</i>	
(280e) PdCu Alloy Nanoparticles As Highly Active Electrocatalysts for Hydrogen Oxidation in Alkaline Electrolyte	200
<i>Yang Qiu, Le Xin, Yawei Li, Ian T. McCrum, Michael Janik, Wenzhen Li</i>	
(280f) Recent Developments in Electrochemical Synthesis of Hydrogen Peroxide	201
<i>Samira Siahrostami</i>	
(296a) Development of a New Generation of Stable, Tunable, and Catalytically Active Nanoparticles Produced By the in-Situ and Ex-Situ Synthesis Methods	202
<i>Jingguang G. Chen, Alexander Orlov, Qiyan Wu, Jiajie Cen, Claron Ridge, Michael Lindsay, Eric A. Stach, Anatoly I. Frenkel</i>	
(296b) Switchable Surfactants for the Preparation of Monodisperse, Supported Nanoparticles and the Effects of Calcination on Nanoparticle Characteristics	203
<i>Kristin Bryant, Steven R. Saunders</i>	
(296c) A Commercially-Viable One-Step Synthesis Method to Prepare MWW Zeolite Nanosheets	204
<i>Yunwen Zhou, Ming-Feng Hsieh, Jeffrey D. Rimer</i>	
(296d) Photocatalytic Inorganic Core Hedgehog Particles	205
<i>Douglas G. Montjoy, Joong Hwan Bahng, Aydin Eskafi, Harrison Hou, Ruiyu Jiang, Nicholas A. Kotov</i>	
(296e) Slowing the Kinetics of Alumina Sol-Gel Chemistry for Controlled Catalyst Overcoating and Improved Catalyst Stability and Selectivity	206
<i>Yuan-Peng Du, Florent Herogue, Jeremy S. Luterbacher</i>	
(296h) One Step, Steady State Catalytic Conversion of Methane to Methanol Using Copper Zeolites: Kinetics and Site Requirements	207
<i>Mark Sullivan, Kimberly Dinh, Randall Meyer, Pedro Serna, Yuriy Roman-Leshkov</i>	
(299a) Photochemical Models for Drug Substance Stability	208
<i>Jose E. Tabora, Michael Smith, Yichen Tan, Thomas La Cruz, Antonio Ramirez, Federico Lora Gonzalez, Thiago Carvalho</i>	
(299b) A Study of Photon Transport in Gas-Liquid Flow: Scalability of Photooxidations from the Micro- to the Milli-Scale	209
<i>Anca Roibu, Rishi Bharadwaj Morthala, Tom Van Gerven, Simon Kuhn</i>	
(299c) Photoredox Iridium-Nickel Dual Catalyzed Decarboxylative Arylation Cross-Coupling: From Batch to Continuous Flow Via Self-Optimizing Segmented Flow Reactor	210
<i>Hsiao-Wu Hsieh, Connor W. Coley, Lorenz M. Baumgartner, Klavs F. Jensen, Richard I. Robinson</i>	
(299d) Studies Toward Scalable Photochemical Reactions in Flow	211
<i>Emily Corcoran, Francois Levesque, Jonathan P. McMullen, John R. Naber</i>	
(299e) Improving Reactor Design for Scaling-up Photoredox Reactions in Flow	212
<i>Eric G. Moschetta, Kaid Harper, Shailendra Bordawekar, Steven J. Wittenberger</i>	
(299f) Photon Mediated Coupling Reactions Using Copper Nanocatalysts - Molecular Mechanisms on Homo Coupling and Hetero Coupling Activity	213
<i>Ravi Teja, Andishaeh Dadgar, Farshid Mohammadparast, Marimuthu Andiappan</i>	
(311a) The Impact of Shale Gas and Oil on the Chemical Industry	214
<i>Jeffrey J. Sirolo</i>	
(311b) Sustainable Energy and Chemicals: Past, Present, and Future	215
<i>Joseph B. Powell</i>	
(311c) Disruptions: What the Future May Hold	216
<i>Scott F. Mitchell</i>	
(311d) Geopolitical Factors Influencing the Evolution of the Chemical Industry	217
<i>David West</i>	
(311e) Agility & Resilience: How to Maintain Career Competitiveness in the Changing Chemical Industry	218
<i>Antonis Papadourakis</i>	
(316a) Single-Molecule Characterization of Czyme Protein Modules Adsorption to Multivalent Glucan Polymers like Cellulose	219
<i>Shishir Chundawat, Bhargava Nemmaru, Mark Hilton, Markus Hackl, Cesar Lopez, Gnana Gnanakaran, Matthew Lang</i>	
(316b) Combinatorial Experimental and Computational Approach for the Effective Entrapment of Glucose Oxidase in Hyaluronic Acid Nanogels	220
<i>Jordan Chapman, Ahmed E. Ismail, Cerasela Zoica Dinu</i>	
(316c) Spatiotemporal Dynamics from a Classic Enzyme Cascade with Self-Governing Substrate Competition	221
<i>Yifei Zhang, Stanislav Tsitkov, Henry Hess</i>	
(316d) Uncovering the Quantum Mechanical Origins of Enzymatic Catalysis with Systematic QM/MM Methods and Accelerated, Large-Scale Electronic Structure	222
<i>Heather J. Kulik, Zhongyue Yang, Rimsha Mehmood, Mengyi Wang, Helena Qi</i>	
(316e) Towards Scalable Production of Enantiomerically Pure Amines: Enzyme Mechanism and Kinetics	223
<i>Robert D. Franklin, John M. Robbins, Joshua Whitley, Andreas S. Bommarius</i>	
(316f) Construction of Artificial Metalloenzyme Catalyst and the Study of Size Effect	224
<i>Xiaoyang Li Jr., Jun Ge</i>	
(316g) Functionalized Magnetic Graphene Oxide Sheets for Efficient Cota Laccase Immobilization	225
<i>Chunzhao Liu</i>	

(322a) Catalytic Aromatization of Bio-Derived Liquid Under Methane Environment	226
<i>Aiguo Wang, Danielle Austin, Hua Song</i>	
(322b) Wave LiquefactionTM Processing of Carbon Materials for the Production of Value-Added Chemicals and Feedstocks: Spectroscopic Diagnostics and Material Characterization	227
<i>Randy Vander Wal, Arupananda Sengupta, Madhu Singh, Kurt Zeller, George Skoptsov</i>	
(322c) Hydrocarbon Chain Growth Via a Nonthermal Electrical Plasma Microreactor	230
<i>Ian Reddick, Goran Jovanovic, Alexandre Yokochi, Nick Auyeung, Matthew Young Coblyn, Yu Miao, Omar Mohamed, Adam Shareghi, Andrew Traverso, Anthony Pyka</i>	
(322d) Combined Experimental and Density Functional Theory Studies on the Modified SrTiO₃ Catalysts for Oxidative Coupling of Methane	231
<i>Seo Yeon Lim, Jae-Wook Choi, Dong Jin Suh, Kwang Ho Song, Hyung Chul Ham, Jeong-Myeong Ha</i>	
(322e) Process Technology Assessment for Mega Scale Projects	232
<i>Yizu Zhu, Mohammad Shafiei</i>	
(327a) Pd As an Oxidation State Modifier and Cocatalyst for the Re-Catalyzed Heterogeneous Deoxydehydration	233
<i>Andreas Heyden, Yongjie Xi</i>	
(327b) First-Principles Modeling of Single-Atom Catalysis: CO Oxidation over Atomically Dispersed Pt on CeO₂	234
<i>Yifan Wang, Ya-Qiong Su, Jin-Xun Liu, Ivo Filot, Konstantinos Alexopoulos, Dionisios G. Vlachos, Emiel Hensen</i>	
(327c) DFT and Microkinetic Comparison of Pt, Pd and Rh(111) for Catalytic Ammonia Oxidation	235
<i>Hanyu Ma, William F. Schneider</i>	
(327d) Face-Centered Tetragonal Pt Alloys of Fe & Co As Potential Catalysts for ORR	236
<i>Shubham Sharma, Andrew A. Peterson</i>	
(327e) Electronic Effects on Open Framework Material-Encapsulated Metal Nanoparticles (NP@OFM) and Implications on Catalysis	237
<i>Benjamin Schweitzer, Chloe Archuleta, Diego Gomez Gualdrón</i>	
(327f) CO₂ Reduction on Ligand-Protected Au Nanoclusters	238
<i>Giannis Mpourmpakis, Natalie Austin</i>	
(327g) Mechanistic Insights into Non-Oxidative Ethane Dehydrogenation on Pt-Based Catalysts Via First-Principles Microkinetic analysis	239
<i>Talin Avanesian, Dionisios G. Vlachos</i>	
(327h) Predictive Model for Catalyst Effect of Photo-Induced and Copper-Catalyzed Atom Transfer Radical Polymerization (ATRP) Reaction	240
<i>Cheng Fang</i>	
(334b) Metal-Modified Transition Metal Nitride Electrocatalysts for Oer, HER, and Other Reactions	241
<i>Brian M. Tackett, Jingguang G. Chen, Qian Zhang</i>	
(334c) Combining Electrochemistry and Surface Science to Identify Electrocatalytic Structure-Property Relationships	242
<i>Douglas R. Kauffman, Xingyi Deng, Dominic Alfonso, Junseok Lee, Dan C. Sorescu, Christopher Matranga</i>	
(334d) Active Structures and Species of Modified Oxide Catalysts for the Oxygen Evolution Reaction (OER)	243
<i>Bruce E. Koel</i>	
(334e) Lowering the Charge Overpotentials in Li-O₂ Battery By Tailoring the Oxygen Reduction and Evolution Reaction Energetics Using Non-Precious Metal Oxide Electrocatalysts	244
<i>Samji Samira, Ayad Nancy, Eranda Nikolla</i>	
(334f) Density Functional Theory Study of Oxygen Evolution Reaction on Specific Terminated Facets of Perovskite Oxides	245
<i>Nicholas Apodaca, Pabitra Choudhury</i>	
(334g) Core-Shell Nanoparticles for Efficient Oxygen Evolution Electrocatalysis in Alkaline and Acidic Media	246
<i>Alaina Strickler, Maria Escudero-Escribano, Thomas F. Jaramillo</i>	
(350a) Runaway in MICRO-Channel Reactors	247
<i>Sunjeev Venkateswaran, Benjamin Wilhite, Costas Kravaris</i>	
(350b) Cyclohexanone Ammoximation over TS-1 Catalyst without Organic Solvent in a Microreaction System	248
<i>Yunpeng Hu, Dong Chen, Tao Wang Sr., Guangsheng Luo</i>	
(350c) Modeling-Aided and Experimental Approaches for Design of Microreactors Using 3D Printing	249
<i>Haomiao Zhang, Klavs F. Jensen</i>	
(350d) A Study on Catalytic Combustion of Methanol-Air Mixture in Microreactors	250
<i>Neha Yedala, Niket S. Kaisare</i>	
(350e) Nanoemulsion Meets Droplet Microfluidics: Controlled Mass Transport and Applications in Micro- and Nanoparticle Preparation	251
<i>Tonghan Gu, Fan He, Yunfei Zhang, T. Alan Hatton, Saif A. Khan</i>	
(350f) Process Intensification of Sulfuric Acid Alkylation Using a Microstructured Chemical System	255
<i>Liantang Li, Jisong Zhang, Chencan Du, Guangsheng Luo</i>	
(350g) Single-Droplet Flow Chemistry Platform for High-Throughput Studies of Rhodium-Catalyzed Hydroformylation Reactions	256
<i>Cheng Zhu, Keshav Raghuvanshi, Connor W. Coley, Milad Abolhasani</i>	
(352a) Dry Reforming of Methane over Ce_{0.7}Ti_{0.3}O_{2-δ} supported Nickel Catalyst	257
<i>Sachin Nandanwar, Yunkai Zou, Linze Du, Joseph H. Holles, Jing Zhou</i>	
(352b) Controlled Metal@Metal Oxide Core-Shell Structures for Selective Heterogeneous Catalysis	258
<i>Bingwen Wang, Jing Zhang, J. Will Medlin, Eranda Nikolla</i>	
(352c) Protecting the Fe Active Phase from Oxidation Under Hydrodeoxygenation Conditions: Evaluating the Influence of Promoters and External Electric Fields	259
<i>Jacob Bray, Alyssa Hensley, Greg Collinge, Jean-Sabin McEwen</i>	

(352d) Synthesis and Catalytic Testing of Lewis Acidic Nano-MFI Zeolites for Epoxide Ring Opening Reaction with Alcohol	260
<i>Amena Parulkar, Rutuja Joshi, Nitish Deshpande, Alexander Spanos, Nicholas Brunelli</i>	
(352e) Understanding Intramolecular Cooperativity in Acid-Base Silica-Supported Organocatalysts	261
<i>Jingwei Xie, Nathan Ellebracht, Christopher W. Jones</i>	
(352f) Study of Ethanol Decomposition Mechanism over Combustion Synthesized Bimetallic Cu-Co Nanoparticles	262
<i>Anand Kumar, Anchu Ashok, Faris Tarlochan</i>	
(352g) Synergetic Effect of Ultrafine NiCo Bimetallic Alloy Nanoparticles Derived from Bimetal-Organic Frameworks	271
<i>Huanjun Wang, Xiaodan Li II, Xiaocheng Lan III, Tiefeng Wang</i>	
(369a) Introduction to the Chemical Catalysis for Bioenergy Consortium	272
<i>Joshua A. Schaidle</i>	
(369b) Introduction to Catalyst Cost Estimation	273
<i>Frederick Baddour</i>	
(369e) Flow Synthesis: An Improved Path to Market for Nanoparticle Catalysts	274
<i>Noah Malmstadt</i>	
(369f) Capability Highlight: Estimation of Spent Catalyst Value	275
<i>Lesley J. Snowden-Swan</i>	
(380a) Towards Rational Synthesis and Molecular Level Understanding of Pd/Zeolite Passive NO_x Adsorber (PNA) Materials	276
<i>Konstantin Khivantsev, Nicholas Jaegers, Libor Kovarik, Yanran Cui, Franklin (Feng) Tao, Jonathan C. Hanson, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Yong Wang, Feng Gao, Janos Szanyi</i>	
(380b) Sulfur Dioxide Oxidation Studies with Precious Metal Catalysts: Sulfur Surface Species Stability Versus Adsorption Amount Impact on Activity Loss	277
<i>M. S. Wilburn, William S. Epling</i>	
(380c) Kinetic Study of the Reduction and Oxidation Half-Cycles during Selective Catalytic Reduction of NO_x with Ammonia on Cu-SSZ-13	278
<i>Ishant Khurana, Arthur J. Shih, Sichi Li, Casey Jones, Aleksey Yezerets, W. N. Delgass, Jeffrey T. Miller, William F. Schneider, Rajamani Gounder, Fabio H. Ribeiro</i>	
(380d) Pd@CeO₂ Core@Shell Nanoparticles: Enhancing Thermal Stability and Activity in Three-Way Automotive Catalysts	279
<i>Alexander Hill, Chang Yup Seo, Johannes W. Schwank, Andrej Lenert</i>	
(380e) Multi-Scale Modelling of Gasoline Particulate Filters - How the Porous Structure of Filter Affects Its Performance	280
<i>Marek Vaclavik, Marie Placha, Martin Isoz, Martin Leskovjan, Panagiotis Boutikos, Petr Koci, Milos Svoboda, Emily Price, Vladimir Novak, David Thompsett</i>	
(380f) Assessing the Catalytic Applicability of Zirconium and Cerium Oxide Microspheres Prepared By Internal Gelation	281
<i>Jae-Soon Choi, Jack L. Collins, Ercan Cakmak, Michael J. Lance, Rodney D. Hunt</i>	
(380g) Tuning ZSM-11 Catalyst Performance in the Methanol-to-Hydrocarbon Reaction through Controlled Post-Synthesis Modification	282
<i>Thuy T. Le, Heng Dai, Jeffrey D. Rimer</i>	
(384a) 25 by 25: Chemical Engineering in the Next 25 Years	283
<i>Clare McCabe, Phillip R. Westmoreland</i>	
(384b) The Future of Chemical Engineering Itself	284
<i>Phillip R. Westmoreland</i>	
(384e) Accelerating Innovation through Academic-Industrial Partnerships	285
<i>William Liechty, Shawn D. Feist</i>	
(384c) Maximizing Uptime, Efficiency, and Safety of Industrial Operations through Early Risk Detection	286
<i>Ankur Pariyani</i>	
(384d) Gaussian Processes for Hybridizing Analytical & Data-Driven Decision-Making	287
<i>Simon Olofsson, Johannes Wiebe, Marc Peter Deisenroth, Ruth Misener</i>	
(389a) Understanding the Importance of High Coverages in Electro-Catalysed Reduction of NO on Pt-Sn Alloys	290
<i>Siddharth Deshpande, Jeffrey Greeley</i>	
(389b) Probing the Intrinsic Reaction Barriers of HER in Acidic and Alkaline Media Using Electronic Structure Theory	291
<i>Per Lindgren, Georg Kastlunger, Andrew A. Peterson</i>	
(389c) First-Principles Prediction of Activated Carbon Nanostructures for Catalyzing Oxygen Reduction	292
<i>Gregory Hartmann, Gyeong S. Hwang</i>	
(389d) Quantifying Confidence in DFT Predicted Surface Pourbaix Diagrams and Associated Reaction Pathways for Chlorine Evolution	293
<i>Vaidish Sumaria, Dilip Krishnamurthy, Venkatasubramanian Viswanathan</i>	
(389e) A Roadmap for Modeling Single-Site (electro)Catalysts: A Combined Coupled Cluster, DFT and a Classical Force Field Approach	294
<i>Jens Nørskov, Anjali M. Patel, Ambarish Kulkarni</i>	
(389f) The Effect of Electrode Potential on the Stability of Intermediates Involved in Both Electrochemical CO₂ Reduction and Hydrogen Evolution	295
<i>Haochen Zhang, William A. Goddard III, Qi Lu, Mu-Jeng Cheng</i>	
(389g) Trends in Electrochemical Oxygen Reduction and Evolution Activities of Layered Double Hydroxides	304
<i>Zhenghang Zhao, Ambarish R. Kulkarni, Michal Bajdich, Jens Nørskov</i>	

(399a) Adsorption of Organics and Nitrate on Pt Electrodes for Electrochemical Reduction Reactions	305
<i>Nirala Singh, Udishnu Sanyal, Danielle Richards, Jin-Xun Liu, John L. Fulton, Charles T. Campbell, Johannes A. Lercher, Bryan Goldsmith</i>	
(399b) Mechanistic Insights into Selective Hydrogenation of Furfural over Metal Electrodes.....	306
<i>Xiaotong Chadderton, David Chadderton, John Matthiesen, Jean-Philippe Tessonnier, Wenzhen Li</i>	
(399c) Impact of Phenol on the Electrocatalytic Hydrogenation of Carbonyl Compounds on Metal Catalysts	307
<i>Udishnu Sanyal, Katherine Koh, Laura Meyer, Jamie Holladay, Oliver Gutierrez, Johannes A. Lercher</i>	
(399d) Electro-Oxidation of Furans to Value-Added Chemicals	308
<i>Alex Roman, J. Will Medlin, Adam Holewinski</i>	
(399e) Low Energy Electrochemical Oxidation of Waste Lignin on Non-Precious PbO₂/MWNTs Electrocatalyst for Simultaneous Generation of Value-Added Chemicals and Hydrogen	309
<i>Fazel Bateni, John Staser</i>	
(399f) Metal Nitride-Type Cathode Catalysts for Electrocatalytic Ammonia Production.....	310
<i>Seval Gunduz, Dhruva Jyoti Deka, Doruk Dogu, Katja E. Binkley Meyer, John McGrogan, Anne Co, Umit S. Ozkan</i>	
(399g) Selective Hydrogenations in Proton Exchange Membrane Reactor	311
<i>Sarah Carl, Krysta Waldrop, Peter N. Pintauro, Levi T. Thompson</i>	
(399h) Rational Design of Metal Electrocatalysts for Ambient Ammonia Synthesis.....	312
<i>Xiaofeng Feng</i>	
(407b) Breaking the Barriers in Lignin Upgrading Using a Catalytic Funneling Strategy	313
<i>Yuriy Roman-Leshkov</i>	
(407c) How Can Catalysis Enable the Reduction of CO₂ Emissions By the Fuels and Chemicals Industries?	314
<i>Alexis T. Bell</i>	
(407d) Development of New Flow Reactors and Their Application for Rhodium-Catalyzed C-H Activation in Organic Synthesis	315
<i>Chunjae Yoo, Eric G. Moschetta, Kathryn M. Chepiga, Daniel Rackl, Solymar Negretti, Nicholas Brunelli, Ryan Lively, Huw M. L. Davies, Christopher W. Jones</i>	
(407e) Metal Catalysts for Cooperative Activation of Cellulose.....	316
<i>Paul Dauenhauer</i>	
(407g) From First Principles to Chemical Manufacturing of Renewable Chemicals	317
<i>Dionisios G. Vlachos</i>	
(413a) Open Source Controls, Cloud Computing and Paradigm Changes in Laboratory-Scale Reactor Control.....	318
<i>Benjamin Rizkin, Ryan L. Hartman</i>	
(413b) Two-Phase Microreactor Design for the Reactive Extraction of Biomass Derivatives	319
<i>Pierre Desir, Basudeb Saha, Dionisios G. Vlachos</i>	
(413c) Alloy Catalysis Spanning Composition Space	320
<i>Irem Sen, Petro Kondratyuk, Andrew J. Gellman</i>	
(413d) Microfluidic Approaches for Accessing Thermodynamic Properties of Fluid Systems	321
<i>T. Gavaille, Nicolas Pannacci, Ghislain Bergeot, Samuel Marre</i>	
(413f) Converting Biogas to Liquid Fuels By Low Energy Electrical Corona Discharge Processes.....	322
<i>Yu Miao, Ian Reddick, Adam Shareghi, Andrew Traverso, Nicolas AuYeung, Annette Von Jouanne, Goran Jovanovic, Alexandre Yokochi</i>	
(413g) Microenvironment Effect on Reaction Kinetics within Self-Assembled Polymer Nanoreactors.....	323
<i>Andrew Harrison, Tien Vuong, Michael Zeevi, Christina Tang</i>	
(431b) Commercialization Example: Catalytic Indirect Liquefaction of Biomass	324
<i>Joshua A. Schaidle</i>	
(445a) C₂ Oxygenates from Syngas: Understanding and Improving Methanol Carbonylation Using Modified Mordenite Catalysts	325
<i>David Chester Upham, Marat Orazov, Thomas F. Jaramillo</i>	
(445b) Effects of Acid Site Proximity and Confinement in Zeolites on Methanol Dehydration Reaction Mechanisms Prevalent during Low-Temperature Catalysis.....	326
<i>John R. Di Iorio, Steven V. Nystrom Jr., Claire T. Nimlos, Alexander Hoffman, David Hibbitts, Rajamani Gounder</i>	
(445c) Deconvoluting the Competing Effects of Zeolite Framework Topology Versus Diffusion Path Length on Methanol-to-Hydrocarbon Reactions.....	327
<i>Yufeng Shen, Thuy T. Le, Donglong Fu, Joel E. Schmidt, Matthias Filez, Bert Weckhuysen, Jeffrey D. Rimer</i>	
(445d) Kinetic and Mechanistic Study of the Chemistry Involved in the Deactivation of Zeolite Catalysts during Methanol-to-Hydrocarbons Conversion	328
<i>Brandon Foley, Thomas Chen, Matthew Neurock, Aditya Bhan</i>	
(445e) Increasing Btp-X and C₂-C₃ Olefins in Methanol to Aromatics over Shape-Selective Zn-Si-HZSM-5	329
<i>Abhay Zambare, Shi-Shang Jang, David Shan-Hill Wong, John Ou</i>	
(445f) Mechanistic Details of Formic Acid Dehydration on TiO₂ and ZrO₂ Catalysts.....	330
<i>Stephanie Kwon, Ting Chun Lin, Enrique Iglesia</i>	
(445g) Highly Selective Conversion of Methanol to Propylene: Design of a MFI Zeolite with Selective-Blockage of (010) Surfaces.....	331
<i>Dali Cai</i>	
(445h) Selective Oxidation of Methane to Methanol: How to Live with the Selectivity-Conversion Limit	332
<i>Arvin Kakekhani, Allegra A. Latimer, Ambarish R. Kulkarni, Jens Norskov</i>	
(446a) Organotemplate-Free Beta Zeolites: From Zeolite Synthesis to Hierarchical Structure Creation.....	333
<i>Ke Zhang, Sergio Fernandez, Michele L. Ostraat</i>	

(446b) Tuning the Molecular Design of Tertiary Amine Catalysts on Amorphous Mesoporous Silica Supports for Selective Glucose Isomerization and Acid-Base Cooperative Reactions	334
<i>Nicholas Brunelli, Nitish Deshpande, Takeshi Kobayashi, Chi-Ta Yang, Eun Hyun Cho, Mariah Whitaker, Aamena Parulkar, Marek Pruski, Li-Chiang Lin</i>	
(446c) Template Free Synthesis of Palladium Immobilized Ordered Mesoporous Resin for Drug Synthesis on a Chip	335
<i>Mahboubeh Nabavinia, Alexander Hesketh, Philip Wall, Elizabeth Kuhlman, Justin Ryan, Sabrina Rittweger, Matthew Knighton, Amanda Christon, Meagan Schweiger, Bridget Black, Alexis Lawless-Gattone, Iman Noshadi</i>	
(446d) Mesoporous Zeolites Produced By Solid Crystallization and Their Hydrogenation Properties	336
<i>Yuxin Wang, Cody Baxter, Yixin Liao, Shengnian Wang</i>	
(446e) Pillared Two-Dimensional Titanium Silicalite-1 Zeolite: Synthesis, Characterization and Catalytic Applications	337
<i>Wei Wu, Dongxia Liu</i>	
(446f) Synthesis Methods to Influence Framework Al Arrangements in CHA Zeolites and Consequences for NO_x Selective Catalytic Reduction	338
<i>John R. Di Iorio, Sichi Li, Subramanian Prasad, Ahmad Moini, William F. Schneider, Rajamani Gounder</i>	
(446g) Unraveling and Tuning Surface and Catalytic Chemistry of Zr₆O₈ Nodes in Metal Organic Frameworks	339
<i>Dong Yang, Ruiping Wei, Guozhu Li, Qin Wu, Bruce C. Gates</i>	
(448a) Mechanistic Study on C-C Coupling of Acetaldehyde on Partially Reduced CeO_{2-x}(111)	340
<i>Chuanlin Zhao, Ye Xu</i>	
(448b) Transition Metal Oxides As Catalysts in the Diels-Alder Reaction between Furan and Methyl Acrylate	341
<i>Taha Salavati-Fard, Eftherpi Vasiliadou, Glen Jenness, Stavros Caratzoulas, Raul F. Lobo, Douglas J. Doren</i>	
(448c) Design of Solvent Composition for Acid-Catalyzed Reactions of Biomass-Derived Oxygenates Using Molecular Simulation-Derived Observables	342
<i>Alex Chew, Theodore Walker, Huixiang Li, Benginur Demir, Z. Conrad Zhang, George W. Huber, James Dumesic, Reid C. Van Lehn</i>	
(448d) Catalytic Hydrogenation of Carbon Monoxide to Formaldehyde in Functionalized Metal Organic Frameworks: An Investigation of Pathway and Uncertainty	343
<i>Lin Li, Sen Zhang, J. Karl Johnson</i>	
(448e) Theoretical Insights into Catalytic Upgrading of Ethanol over 2D MFI Zeolite	344
<i>Simuck F. Yuk, Junyan Zhang, Mal-Soon Lee, Sneha A. Akhade, Zhenglong Li, Vassiliki-Alexandra Glezakou, Roger Rousseau, Asanga B. Padmaperuma</i>	
(448f) Multicomponent Catalysis: Directing Reaction Pathways for Hydrodeoxygenation of Furfuryl Alcohol at Pd/TiO₂ Interfaces	345
<i>Shyam Deo, Michael J. Janik, J. Will Medlin, Eranda Nikolla</i>	
(448h) Homogeneous Catalysis of Ketene Production By Triethylphosphate	346
<i>Charles J. McGill, Sara Jo Taylor, Phillip R. Westmoreland</i>	
(464a) Cermet-Based Hydrogen Transport Membrane Reactors for Conversion of Methane to Value-Added Chemicals	347
<i>Dolly Chitta, Javier Alvare, Camilo Corredor</i>	
(464b) Experimental and Numerical Study of an Intensified Water-Gas Shift (WGS) Reaction Process Using a Membrane Reactor (MR)/Adsorptive Reactor (AR) Sequence	348
<i>Huanhao Chen, Mingyuan Cao, Secgin Karagoz, Linghao Zhao, Vasilios Manousiouthakis, Theodore Tsotsis</i>	
(464c) Hydrogen Production in Pd-Based Membrane Reactor Via Reforming Reactions	349
<i>Simona Liguori, Jennifer Wilcox</i>	
(464d) Na-LTA Membranes with High Water Selectivity for Dimethyl Ether Production in a Catalytic Membrane Reactor	350
<i>Huazheng Li, Weiwei Xu, Qiaobei Dong, Fanglei Zhou, Syed Z. Islam, Surya Padinjarekutt, Miao Yu, Naomi Klinghoffer, Shiguang Li, Xinhua Liang</i>	
(464e) PDMS/Ceramic Composite Membrane in Glycerol Fermentation-PV Coupled Process for Biobutanol Production	351
<i>Haipeng Zhu, Jianwei Yuan, Tianpeng Chen, Fengxue Xin, Min Jiang, Gongping Liu, Wanqin Jin</i>	
(464f) Thermochemical Stability of ZIF Membranes for Membrane Reactor Applications	352
<i>Seungju Lee, Jaesung Kim, Doohwan Lee</i>	
(464g) Enhancing CO₂/CH₄ Separation Performance and Mechanical Strength of Mixed-Matrix Membrane Via Combined Use of Graphene Oxide and ZIF-8	353
<i>Wen Li, Samarasinghe Arachchige Sulashi Chathushka Samarasinghe, Tae-Hyun Bae</i>	
(467a) Oscillations and Hysteresis during Hydrocarbon Oxidation on a Diesel Oxidation Catalyst	354
<i>Oxford Peng, Michael Harold, Dan Luss</i>	
(467b) Large Eddy Simulations of Reaction Plumes and Micromixing	356
<i>John A. Thomas, Brian Devincents, Kevin Smith</i>	
(467c) Multi-Scale Modeling of an Annular Structured Catalytic Reactor for Steam Methane Reforming	357
<i>Florent Minette, Juray De Wilde</i>	
(467d) Ignition-Extinction Analysis of Methane Oxidative Coupling in Packed Bed Reactors	358
<i>Zhe Sun, David West, Vemuri Balakotaiah</i>	
(467e) Forced Periodic Reactor Operation with Simultaneous Modulation of Two Inputs: Nonlinear Frequency Response Analysis and Experimental Demonstration	359
<i>Mathias Felischak, Daliborka Nikolic, Menka Petkovska, Andreas Seidel-Morgenstern</i>	
(467f) Analysis of Flow Distribution and Reactions in a Closed Coupled Diesel Oxidation Catalyst	360
<i>Nishithan Balaji, Niket S. Kaisare, Preeti Aghalayam</i>	

(544a) Bifurcation Analysis of Coupled Homogeneous-Heterogeneous Reactions in Monoliths	361
<i>Bhaskar Sarkar, Balakotaiah Vemuri</i>	
(472a) Hydrodechlorination of 1,2-Dichloroethane over Ag-Pd Catalysts Prepared By Controlled Surface Reactions	362
<i>Madelyn R Ball, Eric Stangland, Manos Mavrikakis, James A. Dumesic</i>	
(472b) Science of Shape-Controlled Synthesis of Metallic Nanoparticles	364
<i>Zhifeng Chen, Robert M. Rioux, Ji Woong Chang, Suprita Jharimune, Choumini Balasanthiran</i>	
(472c) Facile Novel Synthesis and Characterization of Gold-Copper Bimetallic Nanoclusters for Applications in Oxidation Catalysis	365
<i>Joseph Brindle, Michael M. Nigra</i>	
(472d) Atomic Layer Deposited Pt-Co Bimetallic Nanoparticles for Selective Hydrogenation	366
<i>Xiaofeng Wang, Yuzi Liu, Xinhua Liang</i>	
(472e) Facile Synthesis of 2D Molybdenum Carbide Nanosheets	367
<i>William P. Mounfield III, Yang Shao-Horn, Yuriy Roman-Leshkov</i>	
(472f) Identification of Optimally Stable Nanoparticle Geometries Via Mathematical Optimization and Density-Functional Theory	368
<i>Natalie M. Isenberg, Zihao Yan, Michael G. Taylor, Christopher L. Hanselman, Giannis Mpourmpakis, Chrysanthos E. Gounaris</i>	
(472g) Niau Single Atom Alloys for the Oxidative Coupling of Methacrolein with Methanol	369
<i>Antonios Trimpalis, Georgios Giannakakis, Junjun Shan, Sufeng Cao, Maria Flytzani-Stephanopoulos, Zhen Qi, Juergen Biener</i>	
(475a) Oxidation of Lignin-Rich Residue from Deacetylation, Mechanical Refining, and Enzymatic Hydrolysis of Lignocellulose	370
<i>Jacob S. Kruger, David Brandner, Camille Amador, Gregg T. Beckham</i>	
(475b) Origins of Char during Fast-Hydropyrolysis of Biomass to Fuels	371
<i>Abhijit Talpade, Richard Caulkins, Lan Xu, Yuan Jiang, Taufik Ridha, Nathan S. Mosier, Hilka Kenttamaa, Rakesh Agrawal, W. Nicholas Delgass, Fabio H. Ribeiro</i>	
(475c) Reaction Analysis and Kinetics of Propionic Acid Hydrodeoxygenation over Supported Pt and Ru Catalysis	372
<i>Joshua Gopeesingh, Jesse Q. Bond</i>	
(475d) Carbohydrate Stabilization Extends the Kinetic Limits of Chemical Polysaccharide Depolymerization	373
<i>Ydna M. Questell-Santiago, Raquel Zambrano-Valera, Masoud Talebi Amiri, Jeremy S. Luterbacher</i>	
(475e) Tuning Pathways for the Diversification of Biomass-Derived Coumalic Acid- Insights from First-Principles	374
<i>Ashwin Chemburkar, Toni Pfennig, Robert Johnson, Matthew Ryan, Aaron Rossini, Brent H. Shanks, Matthew Neurock</i>	
(475f) Selective Catalytic Production of Polyols from Cellulose-Derived Levoglucosenone	375
<i>Siddarth H. Krishna, Zachary R. Schmidt, James A. Dumesic, George W. Huber</i>	
(475g) Kinetic Studies of Acid Hydrolysis of Linear Polysaccharides from Food Waste	376
<i>Elvis Ebikade, Jonathan Lym, Basudeb Saha, Dionisios G. Vlachos</i>	
(500a) Non-Oxidative Conversion of Methane into Light Hydrocarbons Using Single-Atom Platinum Catalysts	377
<i>Chao Wang</i>	
(500b) Highly Selective Nonoxidative Coupling of Methane (NOCM) over Pt-Bi Bimetallic Catalysts	378
<i>Yang Xiao, Arvind Varma</i>	
(500c) Oxidative Coupling of Methane: The Role of the Tungstate Promoter in Mn-Na₂WO₄	379
<i>Gizem Ozbuyukkaya, G. Vesper</i>	
(500d) Microkinetic Modeling of Direct, Non-Oxidative Conversion of Methane to Value-Added Chemicals over Iron/Silica Catalyst	380
<i>Hilal Ezgi Toraman, Konstantinos Alexopoulos, Dionisios G. Vlachos</i>	
(500e) Co-Aromatization of Methane with Propane over Zn/HZSM-5: The Methane Reaction Pathway and the Effect of Zn Distribution	381
<i>Peng He, Jack Jarvis, Shijun Meng, Hua Song</i>	
(500f) Catalytic Aromatization of Methane: Strategies for Improving Active Chemistry and Stability of the Catalysts	382
<i>Sheima J. Khatib, Mustafizur Rahman, Apoorva Sridhar</i>	
(500g) Performance and Phase Stability Studies of Gadolinium-Doped Barium Cerate in Oxidative Coupling of Methane and the Impact of Zr Doping	383
<i>Valentina Omoze Igenegbai, Randall Meyer, Suljo Linic</i>	
(500h) Effects of Controlled Crystalline Surface of Hydroxyapatite on Methane Oxidation Reactions	384
<i>Su Cheun Oh, Dongxia Liu</i>	
(501a) Pt Encapsulated within Small-Pore Zeolites for Selective H₂ Scavenging during Dehydrogenation of Light Alkanes	385
<i>Haefa Mansour, Enrique Iglesia</i>	
(501b) Spatial Characterization of Solid Acid Catalysts By Reactive Gas Chromatography	387
<i>Paul Dauenhauer, Katherine P. Vinter, Omar A. Abdelrahman</i>	
(501c) Speciation of Liquid Ion-Exchanged Cu into SSZ-13, ZSM-5, and Beta Zeolites	388
<i>Arthur J. Shih, Juan M. Gonzalez, Ishant Khurana, Lucia Perez Ramirez, Andres Pena, Aleksey Yezerets, Rajamani Gounder, Aida Luz Villa, Fabio H. Ribeiro</i>	
(501e) First-Principles Development of Al Proximity Titration Strategy for SSZ-13 Zeolite through Comparison of Divalent Metal Cation Exchange Energy Landscapes	389
<i>Sichi Li, Casey Jones, John R. Di Iorio, Anthony Debellis, Imke Britta Mueller, Rajamani Gounder, William F. Schneider</i>	
(501f) Investigating the Effect of Si/Al Ratio on the Catalytic Activity of Two-Dimensional MFI Nanosheets in Friedel-Crafts Alkylations Employing Bulky Reactants	390
<i>Akshay Korde, Byunghyun Min, Sankar Nair, Christopher W. Jones</i>	

(501g) Improving Methanol-to-Olefins Turnover Capacity of CHA Materials By Controlling Methanol Transfer Dehydrogenation Rates	391
<i>Praveen Bollini, Aditya Bhan</i>	
(504a) Examination of Bronsted and Lewis Acid-Catalyzed Alkane Reactions in MFI Zeolites Using a Hybrid QM/MM Scheme	392
<i>Erum Mansoor, Martin Head-Gordon, Alexis T. Bell</i>	
(504b) First Principles Modeling of Extended Solvent Structures in Defected Microporous Materials and Their Influence on the Kinetics of Lewis Acid Site Speciation	393
<i>Brandon C. Bukowski, Jason S. Bates, Rajamani Gounder, Jeffrey Greeley</i>	
(504c) Computational Screening of Metal-Organic Frameworks for Direct Methane to Methanol Conversion	394
<i>Hieu A. Doan, Benjamin Bucior, Randall Q. Snurr</i>	
(504d) Computational Prediction of the Structure and Catalytic Properties of Copper Zirconium Oxide	395
<i>James Dean, Giannis Mpourmpakis</i>	
(504e) Elucidating the Role of Oxygen Coverage in CO₂ Reduction on Mo₂C	396
<i>Mudit Dixit, Xi Peng, Marc D. Porosoff, Giannis Mpourmpakis, Heather D. Willauer</i>	
(504f) Balancing Reactivity and Stability in Metal Nanoparticle and Alumina Support Systems Via Redox Reactions: A Multiscale Computational and Experimental Approach	397
<i>Matthew Curnan, Henry Ayoola, Matthew McCann, Wissam A. Saidi, Judith C. Yang</i>	
(504h) A Theoretical Examination of Nitrogen Photofixation on Rutile TiO₂(110)	398
<i>Benjamin Comer, Andrew Medford</i>	
(510a) U.S. Department of Energy Early-Stage Alkaline Membrane Fuel Cell R&D (Invited)	399
<i>Simon T. Thompson, Donna Ho, Dimitrios Papageorgopoulos</i>	
(510b) Bifunctional Catalyst Enabled Reversible Fuel Cells for Energy Storage (Invited)	400
<i>Hui Xu</i>	
(510c) Ultra-Low PGM and PGM-Free High-Performance Electrodes for Aemfcs	401
<i>Xiong Peng, Travis Omasta, Emanuele Magliocca, William E. Mustain</i>	
(510d) Addressing Transport Losses in Low-Pt and Pt-Free PEM Fuel Cell Cathodes (Invited)	402
<i>Shawn Litster</i>	
(510e) Electrocatalyst Development for Active and Durable Oxygen Evolution Reaction (Invited)	403
<i>Zhenmeng Peng</i>	
(510f) Mechanistic Insights into the Active Sites and Their Local Environments for Electrocatalytic Reduction Systems (Invited)	404
<i>Matthew Neurock</i>	
(510g) Degradation Mechanisms of PEM Water Electrolysis MEA after Long-Term Operation (Invited)	405
<i>Haoran Yu, Leonard Bonville, Radenka Maric</i>	
(510h) Electrocatalytic Conversion of Energy Molecules with 2D Materials (Invited)	406
<i>Dehui Deng</i>	
(522a) Extracting Transport Independent Kinetics for Vapor Phase Upgrading of Biomass Pyrolysis Vapors over H-ZSM-5	407
<i>Vivek Bharadwaj, Brennan Pecha, Anne Starace, Calvin Mukarakate, Peter N. Ciesielski</i>	
(522c) Resolved-Pore CFD Simulation of CO Oxidation in a Catalyst Layer	408
<i>Behnam Partopour, Anthony G. Dixon</i>	
(522e) DFT and Microkinetic Modeling Study of Ethanol from Syngas on Co₇Pd₆ Nanocluster	409
<i>Anuradha Gundamaraju</i>	
(522g) Establishing Discrete Ising Model for Zeolite Deactivation: Inspiration from the Game of Go	410
<i>Dali Cai</i>	
(535a) Dual Functional Zr-KIT-5 Shows Remarkable Activity for Depolymerization of Corn Stover Lignin into Stable Phenolic Monomers	411
<i>Kakasaheb Nandiwale, Andrew Danby, Anand Ramanathan, R. V. Chaudhari, Bala Subramaniam</i>	
(535b) Reaction Condition Optimization for the Scalability of 1,4-Anhydroerythritol and Xylitol Conversion Via Heterogeneous ReO_x-Pd/CeO₂ Catalysis	412
<i>Blake Macqueen, Elizabeth Barrow, Jochen Lauterbach</i>	
(535c) Selective Tuning of the Glycerol C-O Bond Cleavage Sequence on Copper-Modified Molybdenum Carbide Surfaces	413
<i>Zhexi Lin, Weiming Wan, Salai C. Ammal, Kyung-Eun You, Andreas Heyden, Jingguang G. Chen</i>	
(535d) Oxophilic Metal Oxide Modified Iridium Catalysts for Selective Production of Renewable Hydrocarbons	414
<i>Sibao Liu, Basudeb Saha, Dionisios G. Vlachos</i>	
(535e) Localizing Microwave Heat By Surface Polarization of Titanate Nanostructures for Enhanced Catalytic Reaction Efficiency	415
<i>Tuo Ji, Jiahua Zhu</i>	
(535f) Selective Glucose to Fructose Isomerization over Modified Zirconium UiO-66 in Alcohol Media	416
<i>Matheus Dorneles De Mello, Michael Tsapatsis</i>	
(535g) Production of Biorenewable Monomers - from Fructose to 2,5-Furandicarboxylic Acid	417
<i>Ali Hussain Motagawala, Wangyun Won, David Martin Alonso, Christos Maravelias, James A. Dumesic</i>	
(544a) Kinetics of Palm Oil Ethanolysis	418
<i>Mario Andres Noriega, Paulo Cesar Narvaez Rincon, Juan Guillermo Cadavid</i>	
(544b) Catalytic Conversion of Biomass to Value Added Chemicals and Fuels	419
<i>Amoolya Lalsare, Jianli Hu</i>	

(544c) Utilizing a DMSO-like Material in Presence of Sulfuric Acid for Selective Fructose to 5-Hydroxymethylfurfural Reaction in Water	420
<i>Mariah Whitaker, Nicholas Brunelli</i>	
(544d) Controlled Synthesis of Pt-Sn/Al₂O₃ catalysts and Their Application in the Hydrodeoxygenation of Bio-Based Succinic Acid	421
<i>Patrick Howe, Joshua Gopeesingh, Jesse Q. Bond</i>	
(544e) Liquid-Liquid Microfluidic Flows for the Reactive Extraction of HMF	422
<i>Pierre Desir, Basudeb Saha, Dionisios G. Vlachos</i>	
(544f) Acid Hydrolysis of Glycosidic Bonds in Linear Polysaccharides from Food Waste: Kinetic Studies and Modeling	423
<i>Elvis Ebikade, Jonathan Lym, Basudeb Saha, Dionisios G. Vlachos</i>	
(544g) A Spectroscopic Study on the Glucose and Fructose Mutarotation Reactions in the Presence of Lewis and Bronsted Homogeneous Acids	424
<i>Athanasios Kritikos, Siddharth Panditrao, Pranav Ramesh, George Tsilomelekis</i>	
(544h) A Fundamental Study of Cellulose Hydrolysis in Super Acidic Molten Salt Hydrate Media	425
<i>Natalia Rodriguez Quiroz, Dionisios G. Vlachos</i>	
(544i) Conversion of Kraft Lignin to Value Added Aromatic Based Chemicals	426
<i>Deepak Raikwar, Saptarshi Majumdar, Debaprasad Shee</i>	
(544j) Unraveling Surface State and Composition of Highly Selective Nanocrystalline Ni-Cu Alloy Catalysts for Hydrodeoxygenation of HMF	430
<i>Jing Luo, Matteo Monai, Cong Wang, Jennifer Lee, T. Duchon, Filip Dvorak, Vladimir Matolin, Christopher Murray, Paolo Fornasiero, Raymond J. Gorte</i>	
(544k) Hydrotreating of Biomass Derived Bio-Oil/Bio-Crude	431
<i>Huamin Wang, Daniel Santosa</i>	
(544l) Transesterification of Waste Cooking Oil for Biodiesel Production Using Lithium Metasilicate Prepared from Fumed Silica	432
<i>Dai-Ying Lin, Bing-Hung Chen</i>	
(544m) Modeling Solvation Effects for Deoxygenation Reactions	433
<i>Neeraj Rai, Varsha Jain, Shanmuga Venkatesan, Woodrow Wilson, Jordyn Polito</i>	
(544n) Kinetic of the Esterification of Fatty Acids with Methanol for Biodiesel Production	434
<i>Dario Moreno, Andres Abril, Anderson Imbachi, Luis Miguel Serrano Bermudez, Camilo Monroy-Pena, Carlos A M Riascos, Paulo Cesar Narvaez Rincon, Gustavo Buitrago</i>	
(544o) Understanding Catalytic Bifunctionality of Cu/ZSM5 and Cu/Y Zeolites for Biomass Conversions	435
<i>Jiayi Xu, Quanxing Zheng, Keith L. Hohn, Bin Liu</i>	
(544p) Rapid and Simultaneous Production of Furfural and Cellulose-Rich Residue from Sugarcane Bagasse Using a Pressurized Phosphoric Acid-Acetone-Water System	436
<i>Qiong Wang</i>	
(544q) Analysis of Hydrothermal Liquefaction of Food Waste into Biofuel and Biomaterials	437
<i>Aersi Aierzhati, Yuanhui Zhang, Michael Stablein</i>	
(544r) Fast Pyrolysis of Oil Palm Empty Fruit Bunch (EFB) for Bio Oil Production	438
<i>Rozzeta Dolah, Rohit Karnik, Halimaton Hamdan, Haryanti Yahaya</i>	
(544t) Corncob Residue As a Valuable Resource for the Production of Aromatics	439
<i>Yunfei Bai, Yongdan Li</i>	
(544u) MoO₃-Catalyzed Conversion of Guaiacol into Alkylphenols in Supercritical Ethanol	440
<i>Zewei Ma, Yongdan Li</i>	
(544v) Catalytic Glycosylation of Glucose with Fatty Alcohol over Sulfonated Mesoporous Carbons	441
<i>Wahiba Ramdani, Ayman Karam, Karine Vigier, S. Rio, Anne Ponchel, Francois Jerome</i>	
(544x) Thermo-Catalytic Conversion of Lignocellulosic Biomass to Levoglucosenone and 5-Chloromethyl Furfural in Fluidized Bed Reactor	442
<i>Anurag Parihar, Gil Garnier, Sankar Bhattacharya</i>	
(544y) Mechanocatalytic Depolymerization of Cellulose with Perfluorinated Sulfonic Acid Ionomers	443
<i>Prince N. Amaniampong, Ayman Karam, Karine Vigier, Francois Jerome</i>	
(544z) Pt-Ru/CNTs Electrocatalysts for Direct Methanol Fuel Cell	444
<i>Bahareh Alsadat Tavakoli Mehrabadi, John R. Regalbuta, John Weidner, John R. Monnier</i>	
(544aa) Cheap and Upscalable Process for Atomic Layer Deposition on Powder through Stoichiometric Grafting in Solution	445
<i>Benjamin P. Le Monnier, Frederick Wells, Jeremy S. Luterbacher</i>	
(544ab) Automated Microfluidic Platform for High-Throughput Screening of Rhodium-Catalyzed Hydroformylation	446
<i>Cheng Zhu, Keshav Raghuvanshi, Connor W. Coley, Milad Abolhasani</i>	
(544ac) Atomic-Level Insight into Oxygen Adsorption on (hkl) Platinum Surfaces and Implications for the Reactivity in the Oxygen Reduction Reaction	447
<i>Shiyi Wang, Enbo Zhu, Yu Huang, Hendrik Heinz</i>	
(544ad) Immobilized Group IV Metal Precursors on Acidic Supports for Ethylene Oligomerization	448
<i>Joshua D. Wright, Galiya Magazova, Thomas F. Degnan, Jason C. Hicks</i>	
(544af) CO₂-Triggered Recoverable Metal Nanocatalysts Using Unimolecular Core-Shell Star Copolymers As Carriers	449
<i>Yuchen Zhang, Pingwei Liu, Bo-Geng Li, Wen-Jun Wang</i>	
(544ag) Continuous Ligand-Free Palladium-Mediated Carbon-Carbon Cross-Coupling	450
<i>Jeffrey A. Bennett, Jan Genzer, Milad Abolhasani</i>	

(544ah) Simultaneous Cell Disruption and Semi-Quantitative Activity Assays for High-Throughput Screening of Thermostable L-Asparaginases	452
<i>Xian Zhang Sr., Taowei Yang Sr., Meijuan Xu, Zhiming Rao Sr., Shang-Tian Yang</i>	
(544ai) In Situ Observation of Cu₂O Island Reductive Shrinking on Cu(100) Facet Under Methanol Using Environmental Transmission Electron Microscopy	453
<i>Hao Chi, Christopher M. Andolina, Matthew Curnan, Meng Li, G. Vesper, Judith C. Yang</i>	
(544ak) Thermodynamic Complexity of Sulfated Zirconia Catalyst	454
<i>Naiwang Liu, Li Shi, Di Wu, Alexandra Navrotsky</i>	
(544am) The Influence of Size and Surface Structure of Co₃O₄-Supported Pd Nano-Particles on CO Oxidation Activity	455
<i>Rui Huang, Kyeounghak Kim, Jeong Woo Han</i>	
(544an) Novel in Situ Methods to Resolve the Complex Pathways of Zeolite Crystal Growth Towards the Optimization of Microporous Catalyst Synthesis	456
<i>Madhuresh K. Choudhary, Manjesh Kumar, Rishabh Jain, Jeffrey D. Rimer</i>	
(544ao) Experimental Investigation of Bed Size Effects on the Hydrodynamics of Gas-Solid Fluidized Bed Reactor Via Advance Non-Invasive Measurement Techniques (CT and RPT)	457
<i>Abdelsalam Efhaima Sr., Muthanna H. Al-Dahhan</i>	
(544ap) Comparison between the Activities of Cu/Al₂O₃ and TiO₂ in the Liquid Phase Oxidation of Methanol-Ethanol Mixtures: Development of a Kinetic Model for the Catalyst Preparation	458
<i>Francisco Jose Morales Leal, Javier Rivera De La Rosa, Carlos Javier Lucio Ortiz, Diana Bustos Martinez, David Alejandro De Haro Del Rio, Marco Antonio Garza Navarro, Daniela Xulu Vargas Martinez, Carlos D Garcia</i>	
(544aq) First Principles Study of Active Sites on High Performance PGM-Free ORR Catalyst	470
<i>Gurjyot Sethi, Venkatasubramanian Viswanathan</i>	
(544ar) Investigation of Molecular Properties of Imidazolium-Based Ionic Liquids in the Presence of Cysteine Ligated Iron Porphyrins for Understanding Their Biodegradability	471
<i>Atiya Banerjee, Jindal K. Shah</i>	
(544as) Defect Engineering and Sulfation of MOF-808: Towards the Obtainment of Microporous-Mesoporous Structures with Strong Bronsted Sites for Catalysis Applications	472
<i>Carolina Ardila-Suarez, Victor Baldovino-Medrano, Gustavo Ramirez-Caballero</i>	
(544at) Prediction of Surface Energies for Complex Pt Structures from Coordination Number and Generalized Coordination Number	473
<i>Wen Zhong, Christopher L. Hanselman, Kevin Tran, Chrysanthos E. Gounaris, Zachary Ulissi</i>	
(544au) Understanding the pH Dependence of Reversible Hydrogen Reactions	474
<i>Saad Intikhab, Joshua Snyder, Maureen H. Tang</i>	
(544ax) Yolk-Shell Nanoparticle Functionalization for Heterogeneous Hydroamination	475
<i>Trent R. Graham, Ellis Hammond-Pereira, Andika Rosul, Steven R. Saunders</i>	
(544ay) Exploiting Pore Diffusion in Core@Shell Nanocatalysts	476
<i>Yahui Yang, G. Vesper</i>	
(544az) The Effect of Inert Pellet Size in the Fixed-Bed Reactor for Fischer-Tropsch Synthesis	477
<i>Gi Hoon Hong, Young Su Noh, Ali Alizade Eslami, Hyun Dong Kim, Hyun-Tae Song, Dong Ju Moon</i>	
(544ba) Bifunctional Zeolite-Encapsulated Pt Catalysts for Tandem Aldol Condensation and Hydrogenation of Furfural with Acetone	478
<i>Hong Je Cho, Bingjun Xu</i>	
(544bb) Developing First-Principles Based Embedded Atom Method Potentials for Metal Clusters Using Bayesian Statistics	479
<i>Noushin Omidvar, Siwen Wang, Hongliang Xin</i>	
(544bd) Carbon Sphere Supported Cobalt Catalysts for Fischer Tropsch Synthesis	480
<i>Mahluli Moyo</i>	
(544be) Zirconium Hydroxide-Based Sorptive and Catalytic Textiles	481
<i>Natalie Pomerantz, Erin Anderson, Nick Dugan, Nicole Hoffman, Joe Rossin, Rachel Rossin, Pearl Yip</i>	
(544bf) Synthesis of Nanoporous Zeolite-Y Assisted By an Inexpensive Bifunctional Cationic Polymeric Template	482
<i>Aasif Dabbawala, Yasser Al Wahedi, Marios Katsiotis, Balasubramanian V. Vaithilingam, Stephane Morin, Mikael Berthod, Gnana Pragasam Singaravel, Saeed Alhassan</i>	
(544bg) Simple and Cost-Effective Treatment to Enhance Hydrophobicity of Zeolites	483
<i>Aamena Parulkar, Nitish Deshpande, Nicholas Brunelli</i>	
(544bh) Criteria for a Unique Steady State for Guava Juice Depectinization in a Continuous Stirred Tank Reactor	484
<i>Sourav Sengupta, Sirshendu De</i>	
(544bi) Theoretical Investigation of the Effects of Metal Cations on Oxygen Reduction Reaction in Non-Aqueous Metal-Air Batteries	485
<i>Saurin Rawal, William C. McKee, Ye Xu</i>	
(544bl) Electrodeposited Co-Mo-TiO₂ Composites for the Hydrogen Evolution Reaction	486
<i>Cheng Wang, Elizabeth J. Podlaha-Murphy</i>	
(544bm) Metal Supported Ultrathin Oxide/Oxyhydroxide Thin Films for Oxygen Reduction Reaction	487
<i>Seoin Back, Samira Siahrostami, Michal Bajdich, Jens Norskov</i>	
(544bn) Electrodeposited Fe-Rich, Fe-Ni-Co Thin Films for Oxygen Evolution Reaction	488
<i>Yujia Zhang, Elizabeth J. Podlaha-Murphy</i>	
(544bo) Dual CO Light-Off Effect on Pt/Al₂O₃, Pd/Al₂O₃, Pt/CeO₂/Al₂O₃ and Pd/CeO₂/Al₂O₃ in the Presence of C₃H₆	489
<i>Rudolf Pecinka, Jan Brezina, Marek Vaclavik, Petr Koci</i>	

(544bp) Addressing Electronic Conductivity Limitations in Non-Precious Metal Alloy Electrocatalysts	490
<i>Rituja Patil, Aayush Mantri, James R. McKone</i>	
(544bq) Dual Role of Surfactants in Zeolite Catalyst Synthesis and Optimization	491
<i>Aseem Chawla, Rui Li, Rishabh Jain, R. John Clark, James Stujianto, Jeremy Palmer, Javier Garcia-Martinez, Jeffrey D. Rimer</i>	
(544br) Supported Perovskite Oxides for Low Temperature CO₂ Conversion By Reverse Water-Gas Shift Chemical Looping	492
<i>Bryan J. Hare, Debtanu Maiti, Yolanda A. Daza, Adela E. Ramos, Venkat R. Bhethanabotla, John N. Kuhn</i>	
(544bs) Tuning Parameters for Tertiary Amine Catalysts Grafted on Mesoporous Silica for Knoevenagel Condensation	493
<i>Ashwin Kane, Nitish Deshpande, Aamena Parulkar, Mariah Whitaker, Rutuja Joshi, Pinaki Ranadive, Nicholas Brunelli</i>	
(544bt) The Role of Hydroxyl Groups in Carbon Monoxide Oxidation over Copper-Titanium Dioxide Catalysts	494
<i>Guoqiang Cao, Nan Yi</i>	
(544bu) Applications of Microwave Plasma Catalysis	495
<i>Ashley Caiola, Sarojini Tiwari, Xinwei Bai, Amoolya Lalsare, Jianli Hu</i>	
(544bv) A Facile Approach to Prepare Pt Nanoclusters Encapsulated within the Micropores of Zeolite	496
<i>Lisa Nguyen, Junjun Shan, Hui Wang, Jihong Cheng, John Matsubu, Yizhi Xiang, Fu-Kuo Chiang</i>	
(544bw) Mechanistic Insights into the Role of Zr Dopants in Ceria Based Ketone Oxidation Catalysts	497
<i>Ashutosh Mishra, Craig L. Perkins, Allison Robinson, Vassili Vorotnikov, J. Will Medlin, Eric M. Karp</i>	
(544bx) Stability of Fe and Zn Promoted Mo/ZSM-5 Catalysts for Ethane Dehydroaromatization in Cyclic Operation Mode	498
<i>Brandon Robinson, Xinwei Bai, Victor Abdelsayed, Dushyant Shekhawat, Jianli Hu</i>	
(544bz) The Use of Iron Ore As Fischer Tropsch Synthesis Catalyst	499
<i>Katuchero Ramutsindela</i>	
(544ca) Single Rhodium and Palladium Atoms Anchored in Micropores for Transformation of Methane to Acetic Acid and Methanol Under Mild Condition	500
<i>Franklin (Feng) Tao, Yu Tang, Victor Fung, De-En Jiang, Yuting Li, Weixin Huang, Shiran Zhang, Yasuhiro Iwasawa, Tomohiro Sakata, Luan Nguyen, Xiaoyan Zhang, Anatoly I. Frenkel</i>	
(544cc) Porous Titania Microspheres: Highly-Efficient Catalyst Scaffold for Green Syngas Production	533
<i>Mathew Parker, Zachary Campbell, Jacob Lustik, Daniel Jackson, Seif Yusuf, Fanxing Li, Milad Abolhasani</i>	
(544cd) Controlled Post-Synthesis Modification Enables Tuning of ZSM-11 Catalyst Performance in the Methanol-to-Hydrocarbon Reaction	534
<i>Thuy T. Le, Heng Dai, Jeffrey D. Rimer</i>	
(544ce) Adding Water to the Feed of Formic Acid Decomposition over α-MoC Catalyst on Graphite	535
<i>Yahya Aldoshan, Su Ha, Jake T Gray</i>	
(544cf) Platinum Vs. Ruthenium: A Kinetic Comparison of Vapor-Phase Acetone Hydrogenation	536
<i>Xin Gao, Omar A. Abdelrahman, Jesse Q. Bond</i>	
(544cg) Different Catalytic Behaviors of Pd and Pt Metals in Decalin Dehydrogenation to Naphthalene	537
<i>Kyeounghak Kim, Jeong Woo Han</i>	
(544ch) Exploring the Effect of Chloride-Ion Exposure on CN_x and Fe-N-C Catalysts for Application As Oxygen Depolarized Cathodes in Chlorine Production	538
<i>Deeksha Jain, Kuldeep Mantani, Vance Gustin, Seval Gunduz, Anne Co, Umit S. Ozkan</i>	
(544ci) Surfactant-Templated MOF - 808: Effect of CTAB Incorporation on Final Properties and Catalytic Activity	539
<i>Carolina Ardila-Suarez, I. Mora-Vergara, Victor Baldovino-Medrano, Gustavo Ramirez-Caballero</i>	
(544cj) Diffusion of Light Gases in Nanoporous Gold By Pulsed Field Gradient NMR	540
<i>Amineh Baniani, Evan M. Forman, Marcus Baumer, Sergey Vasenkov</i>	
(544ck) Ice-Templating Fabrication of Hierarchical TS-1 Monoliths with Steam-Assisted Crystallization for Enhanced Benzene Hydroxylation	541
<i>Baoquan Zhang, Luwei Geng, Xiufeng Liu</i>	
(544cl) High-Performance Pt-Based Cathode Catalysts: Novel Carbon Supports and in-Situ Generation of Alloy Structure	542
<i>Mengjie Chen, Gang Wu</i>	
(544cm) Preparation of a SBA-15/Cordierite Monolith Support for Intensified Catalytic Reactions	543
<i>Thiago F. De Abreu, Thiago L. R. Hewer, Martin Schmal, Rita M. B. Alves</i>	
(544cn) Mixed Metal Small Pore Zeolites: Synthesis, Characterization and Catalytic Testing	547
<i>Daniel F. Shantz, Aibolat Koishybay</i>	
(544co) One Preparation Method of High Aluminium-Content Sulfated Zirconia: The Influence of Aluminum Contents and Washing on the Structural Morphology, Acidity and Reactivity	548
<i>Zhiming Ma, Li Shi</i>	
(544cp) Iron Supported on Clinoptilolite (natural zeolites) As a Low-Temperature Fischer-Tropsch Synthesis Catalyst	549
<i>Roick Chikati, Diakanua Nkazi</i>	
(544cq) Imidazolinium Based Porous Hypercrosslinked Ionic Polymers for Efficient CO₂ Capture and Fixation with Epoxides	550
<i>Jing Li, Jiahua Zhu, Jun Wang</i>	
(544cr) Synthesis of Novel Hierarchically Porous ZSM-5-KIT-5 Materials and the Catalytic Performances for Hydrodenitrogenation of Quinoline	551
<i>Qian Meng, Aijun Duan, Cong Liu, Di Hu</i>	

(544cs) Facile Fabrication of Dendritic Mesoporous Silica/Carbon Nanospheres for Selective Adsorptive Desulfurization	552
<i>Cong Liu, Pei Yuan, Meng Qian, Hu Di, Aijun Duan</i>	
(544ct) Controllable Synthesis of Spherical Al-SBA-16 Mesoporous Materials with Different Crystal Sizes and Its High Isomerization Performance for Hydrodesulfurization	559
<i>Hu Di, Aijun Duan, Liu Cong, Meng Qian</i>	
(544cv) Pore Size Effect on the Hydrogenation of Diesters over Ordered Hierarchical Cu/HPS Catalyst	560
<i>Yujun Zhao, Bo Peng, Yue Wang, Shengping Wang, Xinbin Ma</i>	
(544cw) Preparation of Highly Dispersed Iron Species over ZSM-5 with Enhanced Metal-Support Interaction By Freeze-Drying Impregnation	561
<i>Lisong Fan, Dangguo Cheng, Fengqiu Chen, Xiaoli Zhan</i>	
(544cx) Controllable Fabrication and Catalytic Performance of Nanosheet HZSM-5 Films By Vertical Secondary Growth	562
<i>Yajie Tian, Li Wang, Qingfa Wang, Xiangwen Zhang, Guozhu Liu</i>	
(544cy) Suitability of Developing Zeolite Y Catalyst from Ediko Nigeria Clay	563
<i>Esio Oboho, Rasheed Babalola, Etim Bassey</i>	
(544cz) Reaction Conversion of Gases in Plasma Reactors	572
<i>Joseph Toth III, Xiaozhou Shen, Daniel J. Lacks, R. Mohan Sankaran</i>	
(544da) Effect of Fe, Mg, Mo, and Pt Promoters on Ni-Based Catalysts over Al₂O₃-CeO₂ for Oxidative Dehydrogenation of Methane with Carbon Oxide	573
<i>Abbas Jawad</i>	
(544db) Investigating the Effect of Addition of Potassium to the Mo/HZSM-5 during the Non-Oxidative Conversion of Methane to Aromatics	574
<i>Vaidheeshwar Ramasubramanian, Hema Ramsurn, Geoffrey Price</i>	
(544dc) Achieving Low-Cost and Accelerated Living Cationic Polymerization of Isobutyl Vinyl Ether in Microflow System	575
<i>Dan Xie, Yangcheng Lu</i>	
(544dh) Spectroscopic Insights into the Oxidation of Nitric Oxide over [Cu, Zn]-ZSM-5	584
<i>Zachary T. Gentle, Daniel F. Shantz</i>	
(544hm) Catalytic Hydrogenation of Carbon Monoxide to Formaldehyde in Functionalized Metal Organic Frameworks: An Investigation of Pathway	585
<i>Sen Zhang, Lin Li, Jonathan Ruffley, J. Karl Johnson</i>	
(544dd) Benchmarks for CO and CO₂ Adsorption on MnO(100): A Comparison of DFT to Experimental Data	586
<i>Han Chen, Xu Feng, David F. Cox</i>	
(544df) Using Density Functional Theory Calculations to Probe the Activity of Bronsted Acid Sites in Zeolite	587
<i>Michael Zeets, Bin Wang</i>	
(544dg) A Fundamental Understanding of the Surface and Catalytic Chemistry of Transition Metal Ceramics in Deoxygenation	588
<i>Yang He, Siris Laursen</i>	
(544dh) Screening Bimetallic Catalyst for CO₂ Reduction Using Machine Learning and DFT Data	589
<i>Zong Qian Yu, Kevin Tran, Zachary Ulissi</i>	
(544di) Development of an Automatic Catalyst Evaluation System Controlled By a Spreadsheet Software	590
<i>Miyu Hirohara, Ken-Ichiro Sotowa, Toshihide Horikawa, Jesus Rafael Alcantara-Avila</i>	
(544dk) First-Principles Study of Hydrogen Dissociation on Plutonium Hydride	591
<i>Ryan Gotchy Mullen, Nir Goldman</i>	
(544dl) Robust Uncertainty Quantification Framework in Computational Electrochemical Functional Materials Design	592
<i>Venkatasubramanian Viswanathan, Dilip Krishnamurthy, Vaidish Sumaria</i>	
(544dm) Metal-Oxide Supported Pt Catalysts for Oxygen Reduction Reaction: A Density Functional Theory Approach	593
<i>Olga Vinogradova, Dilip Krishnamurthy, Lin Li, Venkatasubramanian Viswanathan</i>	
(544dn) Modelling of Four Phase Continuous Hydrogenation Systems	594
<i>Muzammil Khan, Sunil Joshi</i>	
(544do) High Throughput Alloy Catalysis across Composition Space	595
<i>Nicholas Golio, Irem Sen</i>	
(544dq) Thermodynamic and Kinetic Analysis of $\hat{1}^3$-Valerolactone Ring Opening in Multiphase Reactors	596
<i>Xinlei Huang, Zijian Wang, Jesse Q. Bond</i>	
(544dr) Bayesian Chemisorption Theory of Catalysis	597
<i>Siwen Wang, Hongliang Xin</i>	
(544ds) Using Data Science to Reduce Large Reaction Networks in Catalysis	598
<i>Aini Palizhati, Zachary Ulissi</i>	
(544dt) Effect of Water, pH and Electrochemical Potential on Cl Adsorption on Cr₂O₃ Passive Film	599
<i>Kofi Oware Sarfo, Pratik V. Markute, Zavalsa Quezada Gerardo, O. Burkan Isgor, Yongfeng Zhang, Julie D. Tucker, Liney Arnadottir</i>	
(544du) The Effect of Solvents on the Decomposition of Acetic Acid Using Density Functional Theory and Ambient Pressure XPS	600
<i>Sean Seekins, Kingsley Chukwu, Liney Arnadottir</i>	
(544dv) Density Functional Theory Study of Decarboxylation and Decarbonylation of Acetic Acid over Pd (111)	601
<i>Sean Seekins, Kingsley Chukwu, Liney Arnadottir</i>	

(544dw) The Use of Thermodynamics to Predict Cobalt Catalyst Speciation during Fischer Tropsch Reduction and Reaction	602
<i>Joshua Gorimbo, Diane Hildebrandt</i>	
(544dx) Influence of Salt on Nanozeolite-Y Particles Size Synthesized Under Organic Template Free Condition	603
<i>Hanin Radman, Aasif Dabbawala, Yasser Al Wahedi, Gnana Pragasam Singaravel, Stephane Morin, Mikael Berthod, Saeed Alhassan</i>	
(544dy) Thermodynamics of Sorption in Polyolefins in Gaseous and Liquid Media	604
<i>Martina Podivinska, Lenka Krajakova, Jaromir Ponedic, Juraj Kosek</i>	
(544dz) Modeling the Kinetics of Ethane Oxidative Dehydrogenation Via Chemical Looping	605
<i>Vasudev Pralhad Haribal, Luke Neal, Phillip R. Westmoreland, Fanxing Li</i>	
(544ea) Evaluation of the Benefits of Kinetic Monte Carlo and Microkinetic Modeling for Catalyst Design Studies in the Presence of Lateral Interactions	606
<i>Xiao Li, Lars C. Grabow</i>	
(544eb) Exploring Biocatalyst Design and Process Optimization Using Active Learning and Atomistic Simulations	607
<i>Ashraf Ali, Andrew J Adamczyk</i>	
(544ec) Theoretical Studies on the Gas-Phase Synthesis and Properties of Semiconducting Nanomaterials	608
<i>Yeseul Choi, Andrew J Adamczyk</i>	
(544ed) Analysis of Kinetics in the Ring-Opening Reaction and Decarboxylation of β-Valerolactone and Pentenoic Acids over Zeolite Catalysts	609
<i>Xinlei Huang, Jesse Q. Bond</i>	
(544ee) Kinetic Assessments of the Location and Proximity of Bronsted Acid Sites in MFI Zeolites Containing Boron and Aluminum Heteroatoms	610
<i>Philip M. Kester, Elizabeth E. Bickel, Jeffrey T. Miller, Rajamani Gounder</i>	
(544ef) Equilibrium Analysis of Methylbenzene Intermediates for a Methanol-to-Olefins Process	611
<i>Dali Cai</i>	
(544eh) Computational and Experimental Investigations of Electrochemical CO₂ Reduction on a Well-Defined Model Surface	612
<i>Haochen Zhang, Mu-Jeng Cheng, Qi Lu</i>	
(544ei) A Machine Learning Model for Accelerating Biomimetic Electrocatalyst Discovery	613
<i>Hemanth S. Pillai, Noushin Omidvar, Junwei Luo, Hongliang Xin</i>	
(544ej) One Dimensional (1D) Earth-Abundant Based Nanomaterials As Oxygen Evolution Reaction Electrocatalysts for Acid Mediated Proton Exchange Membrane Based Water Electrolysis	614
<i>Shrinath Ghadge, Oleg Velikokhatnyi, Moni Kanchan Datta, Prashant Kumta</i>	
(544ho) Multivariate Analysis of Biomass Conversion Over Ruthenium Catalyst	617
<i>Xiaoping Chen, Jong-Min Lee</i>	
(544ek) Oxidative Desulfurization of Diesel Fuel Using Vanadium Supported Catalyst on Titanium Nanotube	618
<i>Navid Ranjbar, Mohammad Reza Dehghani, Farhad Banisharif</i>	
(544el) CO Oxidation By Single-Atom Pt Catalyst Anchored to Ni-Doped MgO	619
<i>Debolina Misra, Satyesh Yadav</i>	
(544em) Rapid Cycling to Achieve High NO_x Conversion on Pt/CeO₂/Al₂O₃	620
<i>Zhiyu Zhou, Michael Harold, Dan Luss</i>	
(544en) Effect of Al₂O₃ supported Co and Fe Catalysts on Synthesis of Ammonia from CH₄ and N₂ Using Microwave Plasma	622
<i>Sarojini Tiwari, Xinwei Bai, Jianli Hu</i>	
(544eo) Effect of Different Metal Oxide Supported Cu Catalysts for 1,2-Propanediol Production Via Glycerol Hydrogenolysis Route	623
<i>Smita Mondal, Prakash Biswas</i>	
(544eq) Effects of Interface Adsorption of Rhodococcus Ruber TH3 Cells on the Biocatalytic Hydration of Acrylonitrile to Acrylamide	626
<i>Mingzhao Guo, Lufan Yang, Yujun Wang, Guangsheng Luo</i>	
(544er) Oxidative Desulfurization of Thiophenic Components By Vanadium Substituted Dawson-Type Polyoxometalate Supported Catalysts	627
<i>M Naderi Khomartaji, Mohammad Reza Dehghani, Farhad Banisharif</i>	
(544es) Quasi-2D Pd/Pt Nanoclams for CO₂ Reduction in Tandem with Microbial Communities	630
<i>Andrew B. Wong, Frauke Kracke, Antaeres Antoniuk-Pablant, Alfred M. Spormann, Christopher Hahn, Thomas F. Jaramillo</i>	
(544eu) Impact of Polymer-Based Protein Engineered α-Chymotrypsin on Enantioselective Transesterification in Organic Media	631
<i>Hironobu Murata, Stefanie Baker, Yue Sun, Krzysztof Matyjaszewski, Alan Russell</i>	
(544ev) Direct Synthesis of Dimethyl Ether By CO₂ Hydrogenation over a High Active CuO/ZnO/ZrO₂/Al₂O₃ and HZSM-5 Bifunctional Catalyst	632
<i>Shoujie Ren, Weston R. Shoemaker, Xiaofeng Wang, Zeyu Shang, Naomi Klinghoffer, Shiguang Li, Miao Yu, Xinhua Liang</i>	
(544ew) Indirect Oxidation of Glucose to Glucuronic Acid Using Pd-Decorated Au Catalysts	633
<i>Yiyuan Yin, Li Chen, Z. Conrad Zhang, Michael S. Wong</i>	
(544ex) CO₂ Hydrogenation with Ni/MgO Catalysts	634
<i>Astrid Loder, Susanne Lux, Georg Baldauf-Sommerbauer, Matthaues Siebenhofer</i>	
(544ey) Enhancement of Mo/ZSM-5 Catalysts in Methane Aromatization By Addition of Fe Promoters and By Reduction/Carburization Pretreatment	635
<i>Apoorva Sridhar, Mustafizur Rahman, Sheima J. Khatib</i>	

(544fa) The Production of H₂-Rich Gas over SiC Modified Calcium-Aluminate Support Nickel Catalyst for Steam Reforming of Methane	636
<i>Young Su Noh, Gi Hoon Hong, Ali Alizade Eslami, Hyun-Tae Song, Seol A Shin, Hyun Dong Kim, Kwan-Young Lee, Dong Ju Moon</i>	
(544fb) Non-Oxidative Direct Conversion of Methane over Fe(C)SiO₂ Catalyst with Controlling Radical-Based Reaction	637
<i>Seung Ju Han, Yong Tae Kim</i>	
(544fc) Exploring a Tandem Chemocatalytic Route from Syngas to Ethanol	638
<i>Marat Orazov, David Chester Upham, Thomas F. Jaramillo</i>	
(544fd) Dry-Reforming of Methane over M/Ni-M/Al₂O₃-CeO₂ (M =Pt, Fe, Mg, and Mo) Catalysts	639
<i>Abbas Jawad, Fateme Rezaei, Ali Rownaghi</i>	
(544fe) Mechanistic Insights into the Prins Condensation of Formaldehyde with Butene Isomers over H-[Al]-ZSM5 Catalyst	640
<i>Sha Li, Efterpi Vasiliadou, Raul F. Lobo, Dionisios G. Vlachos, Stavros Caratzoulas</i>	
(544ff) Catalytic Reforming of Aqueous Methanol Using Double Cylinder Type Reactor	641
<i>Daisuke Kobayashi, Mitsuyuki Hagiwara, Shin Kobayashi, Atsushi Shono, Yasukazu Saito</i>	
(544fg) Molybdenum Enhanced the Catalytic Activity of Nickel Supported Alumina Catalyst for Hydrodeoxygenation of Stearic Acid	642
<i>Pankaj Kumar</i>	
(544fh) Methane Decomposition for the Production of CO_x-Free Hydrogen and All Base Growth Carbon Nanotubes over Transition Metal Aerogel Catalysts	643
<i>Bingying Gao, I.-Wen Wang, Lili Ren, Hanjing Tian, Jianli Hu</i>	
(544fi) Studies on Fischer-Tropsch Synthesis over Co/Ru/Me-Apso-34 Catalyst	644
<i>Hyun Dong Kim, Gi Hoon Hong, Ali Alizade Eslami, Young Su Noh, Hyun-Tae Song, Ghaffari Saeidabad Nasim, Dong Ju Moon</i>	
(544fj) Methane Decomposition for Carbon Nanotubes and CO_x-Free H₂ over Fe-Based Catalysts on Different Supports	645
<i>I-Wen Wang, Ayillath K. Deepa, Bingying Gao, Hanjing Tian, Jianli Hu</i>	
(544fk) Temperature Programmed Surface Reaction and in-Situ IR Studies of the Oxidative Scission of Methyl Ketones over γ-Al₂O₃ supported Vanadium Oxide	646
<i>Ran Zhu, Siwen Wang, Jesse Q. Bond</i>	
(544fl) Trireforming of Methane for the Production of Syngas over Fe@MWCNT/Co Catalysts	647
<i>Camila Emilia Figueira, Martin Schmal, Reinaldo Giudici, Rita M. B. Alves</i>	
(544fm) A Comparative Study of Nickel Impregnated ZrAlOx Catalysts for Hydrogen Gas Production Via Reforming of Methane	648
<i>Ali Alizade Eslami, Seol A Shin, Hyun Dong Kim, Hyun-Tae Song, Young Su Noh, Gi Hoon Hong, Ghaffari Saeidabad Nasim, Dong Ju Moon</i>	
(544fn) Dehydroaromatization of Ethylene over Metal-ZSM-5 Catalysts	649
<i>Yunwen Zhou, Ming-Feng Hsieh, Hari Thirumalai, Lars C. Grabow, Jeffrey D. Rimer</i>	
(544fp) PtO_x and PdO_x Formation during NO Oxidation on Diesel Oxidation Catalysts	650
<i>Panagiotis Boutikos, Adela Buzkova Arvajova, Marek Vaclavik, Petr Koci</i>	
(544fq) Catalytic Activity of Magnetic Nanoparticles Activated Via RF Induction Heating	653
<i>Natalia Da Silva Moura, Pragathi Darapaneni, Kerry M. Dooley, James A. Dorman</i>	
(544fr) Structure/Redox/Reactivity Properties of Dispersed Vanadium Species on TiO₂ for the Oxidative Dehydrogenation of Propane with CO₂	654
<i>Hedun Wang, George Tsilomelekis</i>	
(544fs) Nanostructured Metal Nitrides and Carbides for Industrial & Environmental Catalysis	655
<i>Kenneth L. Roberts</i>	
(544ft) Hydrogenation of Phenol to Cyclohexanone Via Tubular Nanofiber Supported Catalyst	656
<i>Lin Pan, G. G. Chase</i>	
(544fv) Oxidative Steam Reforming of Methanol over Cu-Zn-Al Oxides for the Production of Hydrogen	657
<i>Xiao Huang, Shuirong Li, Yun-Quan Liu</i>	
(544fw) Ni-Mo₂C: A Highly Active Catalyst for Partial Oxidation of Jet Fuel	658
<i>Qusay Bkour, M. Grant Norton, Su Ha</i>	
(544fx) CO₂-Free Hydrogen Production from Crude Oil through Microwave-Assisted Catalytic Deep Dehydrogenation	659
<i>Yuqiang Yan, Sergio Gonzalez-Cortes, Benzheng Yao, Fahai Cao, Tiancun Xiao, Peter P. Edwards</i>	
(544fy) Metal-Promoted Dehydroaromatization of Ethylene over ZSM-5 Catalysts	660
<i>Yunwen Zhou, Ming-Feng Hsieh, Hari Thirumalai, Lars C. Grabow, Jeffrey D. Rimer</i>	
(544fz) Decolouration of Dye Solutions By Oxidation with H₂O₂ in the Presence of Modified Natural Zeolites	661
<i>Alina Korobeinyk, Stavros Pouloupoulos, Aliya Sataeva, Aigerim Chinakulova, Vassilis J. Inglezakis</i>	
(544ga) Oxidative Dehydrogenation of Propane to Propylene over VO_x/CaO-γ-Al₂O₃	662
<i>Mohammad Mozahar Hossain</i>	
(544hn) Combined Capture and Utilization of CO₂ for Syngas Production over Dual-Function Materials	663
<i>Ahmed Al-Mamoori, Ali Rownaghi, Fateme Rezaei</i>	
(544gc) Recent Developments in Designing Catalysts for Oxygen Reduction Reaction	664
<i>Samira Siahrostami</i>	
(544gd) Advanced Laser-Made Nanocatalysts for Solar Water Splitting	665
<i>Astrid M. Muller</i>	
(544ge) Synthesis and Applications of Heterogeneous Nitrides Nanophotocatalysts	666
<i>Prasaanth Ravi Anusuyadevi, Cyril Aymonier, Samuel Marre</i>	

(544gf) Tuning Cobalt and Nitrogen Co-Doped Carbon Nano Composites for Efficient Oxygen Reduction Reaction	667
<i>Mengran Liu, Yidong Liu, Yong Min</i>	
(544gg) Photocatalytic Degradation of Acid Violet 7 Dye Using a Composite of ZnO/Ppy in Annular Continuos Reactor	668
<i>Diego Alexander Gonzalez Casamachin, Javier Rivera De La Rosa, Carlos Javier Lucio Ortiz, Victor Manuel Ovando Medina, Nancy Elizabeth Davila-Guzman, David Alejandro De Haro Del Rio, Diana Bustos Martinez, Gerardo Antonio Flores Escamilla, Francisco Jose Morales Leal</i>	
(544gh) Degradation of Phenol By Heterogeneous Photocatalysis with TiO₂-Modified BLACK MUD Catalysts	684
<i>Vitoria S. Lourenco, Yvan J. O. Asencios</i>	
(544gi) Electrochemical Charge Transfer Kinetics from Constrained Density Functional Theory	688
<i>Robert Warburton, M. Voros, Larry Curtiss, Jeffrey Greeley</i>	
(544gj) Combustion Synthesis of Ptzn Nanoparticle Electrocatalysts for Ethanol Oxidation in Alkaline Medium	689
<i>Md. Abdul Matin, Anand Kumar</i>	
(544gk) Electrochemical Conversion of Amines to Nitro Explosophores for Energetic Materials	690
<i>Brian F. Disalle</i>	
(544gl) Selective Electrochemical Reduction of CO₂ to Ethylene on Nanopores Modified Copper Electrodes in Aqueous Solution	691
<i>Yuecheng Peng</i>	
(544gm) Nanoporous Palladium Alloys As CO Poisoning Suppressing Electrocatalysts for Electrochemical Conversion of CO₂ to Formate	692
<i>Swarmendu Chatterjee, Yawei Li, Joshua Snyder</i>	
(544gn) Electroless Cu-Ni-Mo-P Catalyst for Electrooxidation and Thermochemical Oxidation of Glycerol	693
<i>Egwu E. Kalu, Kayode F Adekunle, Oyidia Elendu, Ikenna J Nzeribe, Thaddeus Amaechi, Joel Sankar, Paul J Ezeani, Yaw D. Yeboah</i>	
(544go) Enhancement of Photocatalytic Activity of Carbon Nitride By Hydrogen Peroxide Under Visible Light: A Closer Inspection on Reaction Intermediates	694
<i>Mathew M. Desipio, Dipendu Saha</i>	
(544gp) Single-Walled Carbon Nanotube Mediated in Situ Electrochemistry	695
<i>Albert Tianxiang Liu, Yuichiro Kunai, Michael Strano</i>	
(544gq) Effect of Lanthanum and Chlorine Doping on Strontium Titanates for the Electrocatalytically-Assisted Oxidative Dehydrogenation of Ethane	696
<i>Dhruba Jyoti Deka, Doruk Dogu, Katja E. Binkley Meyer, Anshuman Fuller, Seval Gunduz, Nathaniel Kramer, Anne Co, Umit S. Ozkan</i>	
(544gr) Catalytic Thiophene Oxidation By Groups 4 and 5 Zeolite BEA with H₂O₂: Mechanistic and Spectroscopic Evidence for the Effects of Metal Lewis Acidity and Solvent Lewis Basicity	697
<i>Daniel T. Bregante, Ami Patel, Alayna Johnson, David Flaherty</i>	
(544gs) Trends in Adsorption of Electro-Catalytic Water Splitting Intermediates on Hetero-Structures of Perovskite Oxides	698
<i>Liang Zhang, Abhinav S. Raman, Aleksandra Vojvodic</i>	
(544gt) Electrically Enhanced Catalytic Transfer Hydrogenation of Acetophenone in a Biphasic System	699
<i>Nan Wang, Lawrence R. Weatherley</i>	
(544gu) Improving Gasoline-Fed Solid Oxide Fuel Cell Performance with Nickel Catalyst Anode	700
<i>Qusay Bkour</i>	
(544gv) Carbonaceous Supports Decorated with Pt-TiO Nanoparticles Using Electrostatic Self-Assembly Method As a Highly Visible Light Active Photocatalyst for CO Photoreduction	701
<i>Afsanehsadat Larimi</i>	
(544gw) A Systematic Experimental Study on Electrochemical Oxidation of Methane over Transition Metals	702
<i>Aditya Prajapati, Meenesh R. Singh</i>	
(544gx) Kinetic Modelling of Simultaneous Photo-Catalytic Degradation of Phenolic Compounds and Reduction of Metal Ions with Nano-TiO₂	703
<i>Aravind Satish, Sharad M Sontakke, Anirban Roy</i>	
(544gy) Electrode Engineering: Modifying the Hydrophilicity of Carbon Paper for Improved Cobalt Phosphide Hydrogen Evolution Catalysts	710
<i>Joel Sanchez, Laurie A King, Thomas F. Jaramillo</i>	
(544gz) Probing the (Photo)Electrochemical Stability of Atomic Layer Deposited Coatings for Solar-Driven Hydrogen Evolution	711
<i>David W. Palm, Alexander Deangelis, Nicolas Gaillard, Thomas F. Jaramillo</i>	
(544ha) Insights into the Surface Chemical and Catalytic Properties of Photocatalysts That Dictate Activity and Product Distribution in CO₂ Photocatalytic Reduction By H₂O	712
<i>Samiksha Poudyal, Morghan Parker, Siris Laursen</i>	
(544hc) Electrochemical Cycling Strategy for Selective C-C Bonded, Acetylene Production from CO₂ or CH₄ Using Water at Atmospheric Pressure	713
<i>Joshua M. McEnaney, Brian A. Rohr, Adam Nielander, Aayush R. Singh, Jens K. Norskov, Thomas F. Jaramillo</i>	
(544hd) Nitrogen-Doped Carbon Nanostructures As Bifunctional Catalysts for Unitized Regenerative PEM Fuel Cells	714
<i>Deeksha Jain, Kuldeep Mamtani, Anne Co, Umit S. Ozkan</i>	
(544he) High Temperature Co-Electrolysis of CO₂ and H₂O on La_{0.9-x}Sr_xNi_yCo_zFe_{1-y-z}O_{3.1} Type Cathode Catalysts	715
<i>Dhruba Jyoti Deka, Seval Gunduz, Taylor Fitzgerald, Anne Co, Umit S. Ozkan</i>	

(544hf) Highly Durable Pt Fuel Cell Cathode Nanocatalysts Via Nitrogen, Manganese Co-Doped Carbon Derived from Polyaniline Hydrogel	716
<i>Zhi Qiao, Gang Wu</i>	
(544hg) Effects of Electrolyte Composition on Electrochemical CO₂ Reduction	717
<i>Joaquin Resasco, Alexis T. Bell</i>	
(544hh) Hierarchical, Titanium/Titania Electrocatalyst for Water Electrolysis	718
<i>Patricia Taboada-Serrano, Xiang Li, Costas Tsouris</i>	
(544hi) Interaction of Thiol Ligands with Gold and Its Effect on Electrocatalytic CO₂ Reduction	719
<i>Xun Cheng, Yuxin Fang, John C. Flake, Ye Xu</i>	
(544hj) Enhanced CO₂ Electroreduction to CH₄ and C₂H₄ Via Selective Proton Transfer	720
<i>Marcel Schreier, Yogesh Surendranath</i>	
(582a) Reaction Kinetics of Moisture-Reactive Materials for Experimental Validation of a Model for Water Vapor Reaction, Sorption, and Diffusion in Polymers	721
<i>Jennifer M. Knipe, Hom Sharma, Justin Serrine, April M. Sawvel, Yunwei Sun, Elizabeth Glascoe</i>	
(582b) Advances in Organophotocatalysis: Reaction Mechanisms and Applications in Organic and Polymer Synthesis	722
<i>Alan Aguirre-Soto</i>	
(582c) Synthesis and Characterization of Cyclic Poly(vinylmethylsiloxane)-b-Poly(methyl methacrylate)s	723
<i>Baraka S Lwoya, Md Fakar Uddin, Sourav Chatterjee, Saeed Behzadinasab, Julie N. L. Albert</i>	
(582d) Controlled Synthesis of Hyperbranched Polymers Via Semibatch Atom Transfer Radical Copolymerization	724
<i>Mingjiang Zhong, Feng Li, Mengxue Cao, Yujun Feng</i>	
(582e) Tuning Compositional Drift in the Bulk Living Copolymerization of Styrene and Isoprene	725
<i>Bryan S. Beckingham, Sneha B Chakrapani</i>	
(582f) Catalytic Emulsion Polymerization of Ethylene	726
<i>Damien Guironnet</i>	
(582g) Peptide Hydrolysis and the Prebiotic Origin of Functional Peptides	727
<i>Yi Sun, Martha A. Grover, Charles Liotta</i>	
(582h) D-Optimal Estimation of Polyolefin Polymerization Rate Constants Using Experimental Residence Time Studies in Industrial Pilot Plant Equipment	728
<i>Thomas W. Karjala, Brian Kolthammer, Min Zhang, Pradeep Jain</i>	
(605a) Methane Conversion Using Catalytic Melts to Produce Separable Carbon and Hydrogen or Electrical Power	729
<i>David Chester Upham, Michael Gordon, Horia Metiu, Eric W. McFarland, Zachary Snodgrass</i>	
(605b) NiCe@SiO₂ Multi-Yolk-Shell Nanotube Catalyst for Tri-Reforming of Methane	730
<i>Sunkyu Kim, Nicole Cordonnier, Jochen Lauterbach, Erdem Sasmaz</i>	
(605c) Dynamics and Mechanism of Carbon Filament Formation during Methane Reforming on Supported Nickel Catalysts	731
<i>Samuel L. Leung, Junmei Wei, William L. Holstein, Miguel Avalos-Borja, Enrique Iglesia</i>	
(605e) Carbonate-Catalyzed CO₂ Hydrogenation	734
<i>Amy Frankhouser, Aanindeeta Banerjee, Dianne Xiao, Matthew Kanan</i>	
(605f) Bifunctional Catalysts for CO₂ Conversion to Plastics, Chemicals and Fuels	735
<i>Marc D. Porosoff</i>	
(605g) Support and Promoter Effects on the Activity of Transition Metal Phosphide Catalysts for CO and CO₂ Hydrogenation	736
<i>Melis S. Duyar, Eduardo Valle, Alessandro Gallo, Jonathan Snider, Thomas F. Jaramillo</i>	
(605h) Tuning Ni-Catalyzed CO₂ Hydrogenation Pathways Via Ni-Ceria Support Interactions and Ni-Fe Bimetallic Formation	737
<i>Lea Winter, Jingguang G. Chen</i>	
(606a) Structure-Function Relationships for Non-Precious Bimetallic MOF-Derived Catalysts in Vapor-Phase Furfural Hydrogenation	738
<i>Kristina Golub, Taylor Sulmonetti, Lalit A. Darunte, Christopher W. Jones</i>	
(606b) Cage-Defining Ring: A New Molecular Sieve Structural Indicator for Olefin Product Distribution from the Methanol-to-Olefins Reaction	739
<i>Jong Hun Kang, Stacey I. Zones, Mark E. Davis</i>	
(606c) Ab-Initio modeling of Site Interconversion and Microkinetic Modeling of Lewis Acid Zeolites for Butadiene Synthesis	740
<i>Brandon C. Bukowski, Jason S. Bates, Rajamani Gounder, Jeffrey Greeley</i>	
(606d) Predicting Molecular Adsorption Entropies in Confined Environments	741
<i>Paul Dauenhauer, Omar A. Abdelrahman</i>	
(606e) The Catalytic Consequences of Silanol Densities within Titanium BEA on Alkene Epoxidation with Hydrogen Peroxide	742
<i>Daniel T. Bregante, Alayna Johnson, Ami Patel, Zeynep Ayla, David Flaherty</i>	
(606f) Ring-Expansion Carbonylation of Heterocycles By Bimetallic Ion-Pair Catalysis in Co(CO)₄-Incorporated Cr-MIL-101	743
<i>Hoyoung D. Park, Mircea Dinca, Yuriy Roman-Leshkov</i>	
(606g) Zr Metal-Organic Framework As a Catalyst Support for Solid Acid Catalyzed C-C Bond Isomerization and Disproportionation	744
<i>Sol Ahn, Omar K. Farha, Justin M. Notestein</i>	
(618a) Structure and Activity of Alumina-Supported VO_x/TiO₂ Catalysts	745
<i>Izabela A. Samek, N. Scott Bobbitt, Neil M. Schweitzer, Randall Q. Snurr, Peter C. Stair</i>	

(618b) Controlled Doping of CeO₂-ZrO₂ Nanoparticles to Modify Catalytic Activity	746
<i>Behnam Safavinia, Yuming Wang, Jarod Larriviere, James A. Dorman, Kerry M. Dooley</i>	
(618c) Descriptors for Reactivity and Selectivity of Dioxygen Activation Routes on Metal Oxides	747
<i>Stephanie Kwon, Prashant Deshlahra, Enrique Iglesia</i>	
(618d) Towards the Speciation and Reactivity of Facet-Controlled Vanadium Oxide Catalysts	750
<i>Nicholas Jaegers, Lu Zhang, Berlin Sudduth, Eric D. Walter, Mark Engelhard, Libor Kovarik, Mary Hu, Feng Gao, Huamin Wang, Yong Wang, Jian Z. Hu</i>	
(618e) Selective Hydrodeoxygenation of Furfuryl Alcohol on Doped Metal Oxide Catalysts	751
<i>Jiayi Fu, Weiqing Zheng, Jonathan Lym, Konstantinos Alexopoulos, Alexander V. Mironenko, Dionisios G. Vlachos</i>	
(618f) Understanding the Reactivity of Transition-Metal Oxides for Electrochemical Catalysis	752
<i>Michal Bajdich</i>	
(618g) (001)Î³-Fe₂O₃ and CeO₂/Ag: Good Candidates for the Oxygen Reduction Reactions	753
<i>Giulia Righi, Rita Magri</i>	
(618h) Computational Study of Methane Activation on Î³-Al₂O₃	754
<i>Mudit Dixit, Giannis Mpourmpakis, Mitch Cholewinski</i>	
(622a) Use of in-Situ XAS and TXM Techniques for the Simultaneous Determination of Reaction Kinetics and Structural Evolution of CuO during Sulfidation Reactions.	755
<i>Dante Simonetti, Adam Hoffman, Sara Azzam, Kai Zhang, Yahong Xu, Simon R. Bare, Yijin Liu</i>	
(622b) In-Situ Spectroscopic Evidence for the Mars-Van Krevelen Mechanism in the Rh Single-Atom Catalyzed CO Oxidation	756
<i>Ning Yan</i>	
(622c) Operando PM-IRAS+Raman Spectroscopy for Elucidating Poisoning Mechanisms of Pd-Based Hydrogen Separation Membranes in Complex Reaction Mixtures	757
<i>Casey O'Brien</i>	
(622d) A Near Ambient Pressure (NAP)-XPS Study on Platinum Nanoparticles Supported on Zr-Based Metal Organic Frameworks (MOFs)	758
<i>Reza Vakili, Xiaolei Fan, Alex Walton, Chris Hardacre</i>	
(622e) Operando IR Spectroscopy of Electrocatalyst Surfaces for Temperature-Dependent Methane Adsorption and Selective Oxidation	759
<i>Shu Hu, Zachary Fishman</i>	
(622f) Application of in-Situ x-Ray Absorption Spectroscopy for Next-Generation Batteries	760
<i>Mohammad Norouzi Banis, Xia Li, Tom Regier, Yongfeng Hu, Tsun-Kong Sham, Xueliang Sun</i>	
(622g) In Situ/Operando Reaction Cells: Limitations and Opportunities in the UV-Vis and IR Characterization of Catalysts	761
<i>Priya Srinivasan, Juan J. Bravo-Suarez</i>	
(624a) A Computational Fluid Dynamics Study on Reactor Selection for DNA Origami Folding Kinetics	762
<i>Tianyi Hua, Ryan L. Hartman</i>	
(624b) Rational Design of Mixed Solvent Environments for Acid-Catalyzed Biomass Conversion Reactions: A Combined Approach Using Experiments and Molecular Simulations	763
<i>Theodore Walker, Alex Chew, Huixiang Li, Benginur Demir, Z. Conrad Zhang, George W. Huber, Reid C. Van Lehn, James Dumesic</i>	
(624c) Reactions and Chemical Kinetics of Amino Acids in Hot Compressed Water	764
<i>James D. Sheehan, Phillip E. Savage</i>	
(624d) Functionalization of Cellulose Surfaces Using Dye Anchors and Click Chemistry	765
<i>Christy Wheeler West, Amanda Brown, Charles Moran, Mack Bozman, T. Grant Glover, Kevin N. West</i>	
(638a) Production of Jet Fuel from Coal-Derived Syngas	766
<i>Santosh Gangwal, Venkat Venkataraman</i>	
(638b) Energy Efficient Methane Reforming Enabled By Continuous Manufacturing of Porous Titania Microparticles	767
<i>Zachary Campbell, Matthew Parker, Jacob Lustik, Daniel Jackson, Seif Yusuf, Fanxing Li, Milad Abolhasani</i>	
(638c) Enhanced Methane Conversion in Chemical Looping Partial Oxidation to Syngas Using Copper, Cobalt and Nickel Doping Modification with Density Functional Theory Calculation	768
<i>Mengqing Guo, Lang Qin, Zhuo Cheng, Yan Liu, Liang-Shih Fan</i>	
(638d) Modified Ceria for Low-Temperature Methane Partial Oxidation and Water-Splitting	769
<i>Vasudev Pralhad Haribal, Courtney Paulus, Arya Shafiqfarhood, Fanxing Li</i>	
(638e) Particle-Resolved Simulation of Fixed-Bed Reactors Filled with Complex Particle Shapes - a Validation Study	770
<i>Nico Jurtz, Tobias Henkel, Urvashi Srivastava, Matthias Kraume</i>	
(638f) Dry Reforming of Methane over a Ni-Mo Nanocatalyst	771
<i>Youngdong Song, Ercan Ozdemir, Aldiar Adishev, Saravanan Subramanian, Aadesh X. Harale, Bandar Fadhel, Aqil Jamal, Dohyung Moon, Cafer T. Yavuz</i>	
(638g) Fischer-Tropsch Synthesis over Alumina Supported Cobalt Catalyst in a Fixed-Bed Reactor	772
<i>Aaditya Hari Bharanidharan, Mohammed Muzwar, Pushkala Venkatesh, A. K. Suresh, Udaya Bhaskar Reddy Ragula</i>	
(647a) Modeling of Single Atom Catalysis for CO Oxidation	782
<i>Konstantinos Alexopoulos, Dionisios G. Vlachos</i>	
(647b) Iridium and Rhodium Pair-Site Catalysts Supported on MgO	783
<i>Erjia Guan, Bruce C. Gates</i>	
(647c) Predicting the Single-Site CO Oxidation Reactivity Trends on a Well-Defined Copper Oxide Film	784
<i>Kyle Groden, Alex C. Schilling, Alyssa Hensley, Andrew Therrien, E. Charles H. Sykes, Jean-Sabin McEwen</i>	

(647d) Correlation between Atom-Support Interaction and Catalyst Stability & Activity: Implications from a Series of Heteropoly Acids Based Pt1 Catalysts	785
<i>Ning Yan</i>	
(647e) Strong Electrostatic Adsorption and Cryogenic IR Spectroscopy As a General Synthesis and Characterization Approach for Oxide Supported Single Atom Rh Catalysts	786
<i>Chithra Asokan, Phillip Christopher</i>	
(647f) Theoretical Insights on Boron Nitride-Supported Sub-Nanometer Pd6 Clusters for Formic Acid Decomposition: The Effect of Defects	787
<i>Roberto Schimmenti, Manos Mavrikakis</i>	
(544by) Atomically Dispersed Pt and Pd in Small-Pore Chabazite: Synthesis, Characterization and Application	788
<i>Konstantin Khivantsev, Libor Kovarik, Nicholas Jaegers, Jonathan C. Hanson, Franklin (Feng) Tao, Hristiyan A. Aleksandrov, Georgi N. Vayssilov, Yong Wang, Feng Gao, Janos Szanyi</i>	
(653a) Investigation of the Formaldehyde-Isobutene Prins Condensation over MFI Zeolites	789
<i>Efterpi Vasiliadou, Sha Li, Stavros Caratzoulas, Raul F. Lobo</i>	
(653b) 3D-Printed Monoliths of MFI Zeolite with Hierarchical Porosity for Methanol-to-Olefin Reaction	790
<i>Xin Li, Ali Rownaghi, Fateme Rezaei</i>	
(653c) Influence of Confining Environment Polarity and Active Site Structure on Ethanol Dehydration Catalysis By Lewis Acid Zeolites	791
<i>Jason S. Bates, Rajamani Gounder</i>	
(653d) Dehydroaromatization of Ethylene over Bifunctional Lewis-Bronsted Acid Pairs in Ag-ZSM-5	792
<i>Hari Thirumalai, Unmesh Menon, Yunwen Zhou, Jeffrey D. Rimer, Lars C. Grabow</i>	
(653e) Ethylene Oligomerization to Select Oligomers on Ni²⁺-Containing ETS-10	793
<i>Jay Thakkar, Xinyang Yin, Xuanyi Zhang</i>	
(653f) Hydrodeoxygenation of Biomass Pyrolysis Vapors Using Metal Supported USY Zeolite	794
<i>Julia A. Valla, David P. Gamliel</i>	
(653g) Zeolite Bead Heterogeneous Catalysts for Biomass Upgrading in Monophasic and Biphasic GVL Solvent Systems	795
<i>Joelle Romo, Tara Sundsted, Ting Wu, Jolie Lucero, Moises Carreon, Jesse Q. Bond, Stephanie G. Wettstein</i>	
(654a) Investigating Solid Oxide Membrane Reactors for Direct Methane Conversion to Ethylene and Ethane By Oxidative Coupling	796
<i>Valentina Omoze Igenegbai, Randall Meyer, Suljo Linic</i>	
(654g) Atomistic Design of Propylene Epoxidation Catalysts	797
<i>Zheng Lu, Yong Qin, C. Heath Turner, Yu Lei</i>	
(654c) Investigation of the Effect of Pre-Treatment Methods on the Reactivity of Methane, Steam and Oxygen over NiO/Ce_xZr_{1-x}O₂	798
<i>Yimeng Lyu, Carsten Sievers</i>	
(654d) Influence of Confinement in Pores of M1 Phase Mixed Oxides on Selective Oxidative Dehydrogenation of Ethane	799
<i>Annamalai Leelavathi, Yilang Liu, Sopuruchukwu Ezenwa, Yanliu Dang, Steven Suib, Prashant Deshlahra</i>	
(654e) Alkali-Promoted Mixed Oxide Redox Catalysts for Oxidative Dehydrogenation of Ethane in a Cyclic Redox Scheme	800
<i>Fanxing Li, Yunfei Gao</i>	
(654f) Propane Oxidative Dehydrogenation Catalyzed By Iodine, Bromine, and Halide Salts	801
<i>David Chester Upham, Henrik Kristoffersen, Zachary Snodgrass, Michael Gordon, Eric W. McFarland, Horia Metiu</i>	
(655a) Catalytic Etherification of Glycerol to Glycerol Oligomers in the Presence of Alumina Supported Ca/Sr Mixed Oxides	802
<i>Yi-Chen Shih, Bing-Hung Chen</i>	
(655b) The Role of Copper Stability in Selectively Condensation of Ethanol to Higher Alcohols	803
<i>Mond Guo, Karthikeyan K. Ramasamy</i>	
(655c) Effects of Alloying Pd and Cu on Tandem Dehydrogenation-Aldol Condensation Reactions	804
<i>Konstantinos A. Goulas, Yuying Song, Lars C. Grabow, Dean Toste</i>	
(655d) Lubricant Base Oils Production from Biomass	805
<i>Sibao Liu, Basudeb Saha, Dionisios G. Vlachos</i>	
(655e) Selectivity Control during the One-Pot Conversion of Aliphatic Carboxylic Acids to Linear Olefins through Tandem Hydrogenation/Dehydration	806
<i>Jher Hau Yeap, Bartosz Rozmyslowicz, Jeremy S. Luterbacher</i>	
(655f) Mechanism and Kinetics of Isobutene Production over Zirconia-Supported Zinc Oxides	807
<i>Julie Rorrer, Alexis T. Bell, Dean Toste</i>	
(655g) Catalytic Upgrading of Sugar-Derived Polyols to Glycols in Absence of Externally Added Hydrogen	808
<i>Bin Yin, Xin Jin, Guangyu Zhang, Hao Yan, Chaohe Yang</i>	
(655h) Selective C-C Bond Scission of Primary Alcohols Using Cerium Oxide-Supported Palladium Catalyst	809
<i>Tomoo Mizugaki, Kodai Nitta, Takato Mitsudome, Koichiro Jitsukawa</i>	
(659a) Knowledge Extraction Via Machine Learning from High-Throughput Catalytic Experiments	810
<i>Travis Williams, Katherine McCullough, Jochen Lauterbach</i>	
(659b) Catalyst Characterization from Complex Infrared Spectroscopy: A Machine Learning Approach	811
<i>Joshua Lansford, Dionisios G. Vlachos</i>	
(659c) Heterogeneous Catalysis Kinetic Characterization Via Sparse Graphs	812
<i>M. Ross Kunz, Yixiao Wang, Zongtang Fang, Andrew Medford, Gregory S. Yablonsky, Rebecca Fushimi</i>	
(659d) Bayesian Experimental Design and Mean Field Microkinetic Modeling of Heterogeneous Catalytic Systems	813
<i>Huijie Tian, Srinivas Rangarajan</i>	

(659e) Thermochemistry of Gas-Phase and Surface Species Via Lasso-Assisted Subgraph Selection	814
<i>Geun Ho Gu, Petr Plechac, Jonathan Lym, Dionisios G. Vlachos</i>	
(659f) Theoretical Investigation of the Pt Catalyzed Hydrodeoxygenation of Succinic Acid to 1,4-Butanediol	815
<i>Wenqiang Yang, Osman Mamun, Andreas Heyden</i>	
(659g) Large-Scale Exploration of Perovskites for Oxygen Evolution Via Adaptive Machine Learning	816
<i>Zheng Li, Qinghe Zheng, Noushin Omidvar, Hongliang Xin</i>	
(659h) Prospects for Solving Micro-Kinetic Models with Automatic Differentiation and Regression	817
<i>Andrew Medford</i>	
(664a) Enhancing the Specific Activity of Metal Oxides Using Transition-Metal Dopants	818
<i>Jonathan Lym, Konstantinos Alexopoulos, Jiayi Fu, Weiqing Zheng, Alexander V. Mironenko, Dionisios G. Vlachos</i>	
(664b) First-Principles Kinetic Monte Carlo Simulations of Hydrogen Spillover across the Ru/TiO₂ Interface	819
<i>Xiao Li, Lars C. Grabow</i>	
(664c) Design of Multi-Functional Catalytic Interfaces from First Principles: Modelling Water Gas Shift on Pt/MgO	820
<i>Pushkar Ghanekar, Jeffrey Greeley</i>	
(664d) Interaction of Furan and Benzene Derivatives with Palladium Nanoparticle Catalysts and the Mechanism of Conversion into Biofuels	821
<i>Lesli Mark, J. Will Medlin, Hendrik Heinz</i>	
(664e) Mechanistic Interpretations and Consequences of Hydrogen Spillover in Toluene Hydrogenation Catalysis	822
<i>Ari Fischer, Enrique Iglesia</i>	
(664f) Kinetics and Mechanism of Selective C-Cl Hydrogenolysis By Pd/C Catalysts	823
<i>Jalal Tavara, Mohammed Al-Gharrawi, M. Clayton Wheeler, Thomas J. Schwartz</i>	
(664g) The Influence of Support Acid Sites on Non-Oxidative Dehydrogenation of Ethanol to Acetaldehyde over Supported Cu Catalysts	824
<i>Sergei Hanukovich, Phillip Christopher</i>	
(689a) Characterization of Isolated Pt Atoms on Anatase TiO₂	825
<i>Weiqing Zheng, Jiayi Fu, Jonathan Lym, Konstantinos Alexopoulos, Na Li, Jorge A. Boscoboinik, Dong Su, Dionisios G. Vlachos</i>	
(689b) The Marriage of Activity and Selectivity in the Oxidative and Non-Oxidative Activation of Methane on Gold-Palladium Alloys	826
<i>Quan Do, Hung-Vu Tran, Shengguang Wang, Lars C. Grabow</i>	
(689c) Periodic Trends in Adsorption Energies of Transition Metal Precursors on Reducible Cerium Oxide: Towards Rational Synthesis of Single-Site Catalysts	827
<i>Ahana Mukhopadhyay, Robert M. Rioux</i>	
(689d) Structure of the Highly Reduced CeO₂{111} Surface and Its Interaction with Single Atom Rh	828
<i>George Xu Yan, Yu Tang, Franklin (Feng) Tao, Philippe Sautet</i>	
(689e) Non-Oxidative Dehydrogenation of Ethanol to Acetaldehyde and Hydrogen on Nickel-Gold Single Atom Alloys	829
<i>Georgios Giannakakis, Antonios Trimpalis, Maria Flytzani-Stephanopoulos</i>	
(689f) Synthesis, Characterization and Reactivity of Heteroatom Single Site Pairs for Selective Ethylene Conversion	830
<i>Insoo Ro, Chithra Asokan, Phillip Christopher</i>	
(694a) Selective C-H Bond Activation of Light Alkane Using Metal Phosphide Catalysts	831
<i>Jeonghyun Ko, William F. Schneider</i>	
(694b) Catalytic Upgrading of Olefins Under Methane Environment: Effect of Sulfur Poisons on Catalyst Performance and Reusability	832
<i>Jonathan Harray, Aiguo Wang, Peng He, Hua Song</i>	
(694c) MOF-Derived Catalysts for Propane Dehydrogenation	833
<i>Michele L. Sarazen, Christopher W. Jones</i>	
(694d) DFT Investigation of the Mechanism and Site Requirements for Alkane Dehydrogenation on Transition Metal Sulfide Catalysts	834
<i>Ronak Upadhyay, Lohit Sharma, Jonas Baltrusaitis, Srinivas Rangarajan</i>	
(694e) The Migration of Pt and Its Application in the Activation of C-H Bonds of Ethane	835
<i>Junjun Shan, Hui Wang, Lisa Nguyen, John Matsubu, Yizhi Xiang, Fu-Kuo Chiang, Jihong Cheng</i>	
(694f) Co-Oligomerization of Ethylene and Propylene on Acidic Zeolites: A Microkinetic Model	836
<i>Sergio Vernuccio, Linda J. Broadbelt</i>	
(694g) Transient Kinetics Analysis of Ethane Aromatization over Metal Functionalized ZSM-5 Catalyst	837
<i>Yizhi Xiang, Tingyu Liang, Hossein Toghiani</i>	
(695a) Gas Phase Catalytic Oxidation of Lignin to Produce Phenolic Compounds over Vanadia Catalysts	838
<i>Matthew M. Yung, Calvin Mukarakate, Mark Nimlos, Michael B. Griffin, Seonah Kim, Eric C. D. Tan</i>	
(695b) Mechanistic Study of the Hydrogenolysis of Diaryl Ethers Catalyzed By Heterogeneous Metal Catalysts	839
<i>Meng Wang, Oliver Gutierrez, Donald M. Camaioni, Johannes A. Lercher</i>	
(695c) Palladium-Iron Bimetallic Catalyst: High Activity and Stability for Aqueous Phase Hydrogenations	840
<i>Yan Cheng, Hien N. Pham, Robert L. Johnson, Brent H. Shanks, Abhaya K. Datye</i>	
(695d) Hydrodeoxygenation of Guaiacol over Ni and Mo Nanoparticles Supported on SBA-15 and γ-Al₂O₃	841
<i>Thiago L. R. Hower, Rubens W. S. Lima, Reinaldo Giudici, Martin Schmal, Rita M. B. Alves</i>	
(695e) Hydroprocessing of Biomass-Derived Oxygenates on Metal-Exchanged Zeolites Using Light Alkanes As the Source of Hydrogen	844
<i>Dante Simonetti, Eric Lin</i>	
(695f) Flowthrough Reductive Catalytic Fractionation of Biomass	845
<i>Eric Anderson, Michael Stone, Rui Katahira, Michelle Reed, Gregg T. Beckham, Yuriy Roman-Leshkov</i>	

(695h) Hydrodeoxygenation of Sorbitol to Monofunctional Fuel Precursors over Co/TiO₂	846
<i>Nathaniel Eagan, Joseph P. Chada, Ashley Wittrig, J. Scott Buchanan, George W. Huber, James A. Dumesic</i>	
(699a) Catkit: Symmetry Methods for Automated Generation of Catalytic Structures	847
<i>Jacob R. Boes, Thomas Bligaard</i>	
(699b) Predicting Adsorption Properties on Bimetallic Alloys As a Function of Local Morphology and Atomic Composition	848
<i>Tej S. Choksi, Luke Roling, Frank Abild-Pedersen</i>	
(699c) Insights from Machine Learning on a Large Database of Adsorption Energies	849
<i>Matthew M. Montemore, Robert Hoyt, Ioanna Fampiou, Wei Chen, Tess Smidt, Kai Kohlhoff, Patrick Riley, Efthimos Kaxiras</i>	
(699d) Methods to Exploit Large Datasets in Catalysis	850
<i>Kevin Tran, Zachary Ulissi</i>	
(699e) Generalized Geometric Descriptors for Oxygen Reduction Activity on Transition Metal Sulfides	851
<i>Dilip Krishnamurthy, Venkatasubramanian Viswanathan</i>	
(699f) Quantifying Confidence in DFT Predicted Surface Pourbaix Diagrams at Solid-Liquid Interfaces on Transition Metal Surfaces	852
<i>Olga Vinogradova, Dilip Krishnamurthy, Vikram Pande, Venkatasubramanian Viswanathan</i>	
(699g) Accelerating Inorganic Discovery with Machine Learning and Automation	853
<i>Heather J. Kulik, Jon Paul Janet, Aditya Nandy, Chenru Duan, Stefan Gugler</i>	
(704a) Mechanistic Insights into the Direct Propylene Epoxidation over Au/TiO₂/SiO₂	854
<i>Jingjing Ji, Zheng Lu, Yu Lei, C. Heath Turner</i>	
(704b) Effect of PdCu Alloy Composition on Reactivity and Selectivity for Ethylene Acetoxidation to Vinyl Acetate	855
<i>Zhaoru Zha, Annamalai Leelavathi, Prashant Deshlahra</i>	
(704c) Kinetics of Ethylene Oxidation As a Function of Chlorine Coverage over a Highly-Promoted Ag/α-Al₂O₃ Catalyst	858
<i>James W. Harris, Cha-Jung (Maria) Chen, Aditya Bhan</i>	
(704d) Kinetics of the Oxidative Cleavage of Methyl Ketones over Supported Vanadium Oxide Catalysts	859
<i>Ran Zhu, Siwen Wang, Jesse Q. Bond</i>	
(704e) Low-Temperature Selective Oxidation of Methanol to Formaldehyde over Pt-Bi Bimetallic Catalysts	860
<i>Yang Xiao, Yuan Wang, Arvind Varma</i>	
(704f) Water As Poison for H₂ Activation Sites at Au/TiO₂ Interface: Implications for Prox of H₂ in Water-Gas Shift Streams	861
<i>Sravan Kumar Kanchari Bavajigari, Todd Whittaker, Bert D. Chandler, Lars C. Grabow</i>	
(704g) Influence of Support and Environment on the Structure and Properties of Oxide Supported Isolated Pt Atoms	864
<i>Joaquin Resasco, Leo Derita, Phillip Christopher</i>	
(704h) Effect of Dopants on the Activity and Selectivity in the Oxidative Coupling of Methane over Rare Earth Oxides	865
<i>Andrew S Jones, Helena E. Hagelin-Weaver</i>	
(721a) Characterization of Flow and Heat Transfer Parameters in a Continuous Flow Hydrothermal Liquefaction Reactor	866
<i>Feng Cheng, Travis Le-Doux, Brian Trefitz, Scott Woolf, Sergio Guillen, Jacob Usrey, Cesar A. Martinez Bejarano, Hengameh Bayat, Umakanta Jena, Catherine E. Brewer</i>	
(721b) Hydrothermal Liquefaction of Model Polysaccharides and Polysaccharide-Rich Food-Processing Waste	867
<i>Akhila Gollakota, Azin Padash, John Kaplan, Phillip E. Savage</i>	
(721c) Capturing the Phase Interface Using the Gradient Theory in the Mixing of Hydrocarbons and Supercritical Water	868
<i>Ping He, Arash Azimi, Ashwin Raghavan, Ahmed F. Ghoniem</i>	
(721d) Study of the Catalytic Reactions of Ethylene Oligomerization in Subcritical and Supercritical Media over a Nibea Catalyst	869
<i>Gabriel Seufitelli, Fernando Resende</i>	
(721e) Effect of Heterogeneous Catalysts on Upgrading Quality of Bio-Crude Under Sub- and Super-Critical Water Conditions	870
<i>Kodanda Phani Raj Dandamudi, Connor Copp, Tessa Murdock, Peter Lammers, Shuguang Deng</i>	
(721f) Challenges of Designing a Short Residence Time Hydrothermal Continuous Reactor for Algae Processing	871
<i>Ashani Samaratunga, Mason Martin, Orlando Ayala, Sandeep Kumar</i>	
(721g) Hydrothermal Degradation of Hormones and Antibiotics	872
<i>Nepu Saha, M. Toufiq Reza</i>	
(721h) Influence of Solvents on Metal Contents in Biocrude Oil from Hydrothermal Liquefaction of Microalgae	873
<i>Jimeng Jiang, Phillip E. Savage</i>	
(730a) Catalytic Hydrogenation of Furfural over Rumop: Probing Bimetallic and Compositional Effects on Catalyst Performance	874
<i>Yolanda Bonita, Timothy O'Connell, Jason C. Hicks</i>	
(730c) Etherification of 5-Hydroxymethylfurfural Using Zeolite Catalysts	875
<i>Meredith Allen, Spencer Martell, Akbar Mahdavi Shakib, William M. Gramlich, Brian G. Frederick, Thomas J. Schwartz</i>	
(730d) Mechanistic Insights into the Hydrogenolysis of Levoglucosan over Bifunctional Platinum Silica-Alumina Catalysts in Tetrahydrofuran Solvent	876
<i>Siddarth H. Krishna, Rajeev Assary, Quinn A. Rashke, Zachary R. Schmidt, Larry Curtiss, James A. Dumesic, George W. Huber</i>	
(730e) Hydrothermal Stability of Chloromethyl Polystyrene Based Solid Acid Catalysts and Mechanism of Cellulose Hydrolysis	877
<i>Maksim Tyufekchiev, Jordan Finzel, Pu Duan, Klaus Schmidt-Rohr, Sergio Granados-Focil, Marion Emmert, Michael T. Timko</i>	

(730f) Glycerol Transfer-Hydrogenation of Levulinic Acid Using Ru and Ir Carbene Organometallics Immobilized on Active Hydrotalcites	878
<i>Jacob Heltzel, Kai Wang, Matthew Finn, Evan Sandefur, Adelina Voutchkova-Kostal</i>	
(730g) Paired Electrocatalytic Hydrogenation and Oxidation of 5-Hydroxymethylfurfural for Efficient Production of Biorenewable Monomers	879
<i>Xiaotong Chadderdon, David Chadderdon, Wenzhen Li</i>	
(730h) A Full Furfural Utilization over Ni/SiO₂ Catalysts	880
<i>Sheng-Chiang Yang, Shawn D. Lin</i>	
(732a) Accurate Adsorbate Free Energies from First-Principles	881
<i>Prateek Mehta, Anshumaan Bajpai, Kurt Frey, Andrew Lehmer, Gray Laughlin, William F. Schneider</i>	
(732b) Defining and Counting Site Requirements for Reactions on Curved and Crowded Surfaces	882
<i>David Hibbitts, Abdulrahman S. Almithn, David Flaherty, Jianwei Liu, Enrique Iglesia</i>	
(732c) Tuning the Surface Reactivity of Intermetallic Compounds Towards Carbon, Oxygen, and Hydrogen to Affect CO vs. CO₂ Production in Wet Reforming of Hydrocarbons and Oxygenates	883
<i>Yuanjun Song, Yang He, Siris Laursen</i>	
(732d) Amination of 1-Hexanol over Au-Pd/TiO₂ Catalysts Prepared By Controlled Surface Reactions	884
<i>Madelyn R Ball, Thejas S. Wesley, Keishla R. Rivera-Dones, George W. Huber, James A. Dumesic</i>	
(732e) Structure Sensitivity Analysis of Propane Dehydrogenation(PDH) on Palladium Alloys	887
<i>Ranga Rohit Seemakurthi, Fabio H. Ribeiro, Jeffrey Greeley</i>	
(732f) Adsorption and Reaction of Furfuryl Alcohol on Pt(111): A Comparison Study to Pd(111)	888
<i>Lesli Mark, Alexander H. Jenkins, Hendrik Heinz, Will Medlin</i>	
(732g) Kinetics and Mechanism of Aspartic Acid Adsorption and Its Explosive Decomposition on Cu(100)	889
<i>Burcu Karagoz, Aaron Reinicker, A. J. Gellman</i>	
(732h) Density Functional Theory Study of the Effect of Step Edges on $\hat{\pm}$-Fe₂O₃ Surfaces on Cl-Surface Interactions and the Cl-Induced Depassivation Process	890
<i>Qin Pang, Hossein Dormohammadi, O. Burkan Isgor, Liney Arnadottir</i>	
(736a) Experimental and Modeling Study of Passive NO_x Adsorption: Pd-Exchanged-ZSM-5	891
<i>Mugdha Ambast, Kyle Karinshak, Michael Harold</i>	
(736b) Kinetics of the Solid-Liquid Transesterification to Produce Sucrose Esters Using Sodium Stearate As Contacting Agent	894
<i>Maria F. Gutierrez, Alvaro Orjuela, Tapio Salmi, Dmitry Yu. Murzin</i>	
(736c) Model-Based Equipment Design for the Biphasic Production of 5-Hydroxymethylfurfural in a Tubular Reactor	895
<i>Maximilian Aigner, Andreas Jupke, Daniel Roth, Julia Rubkamp</i>	
(736d) Exploring the Contribution of Liquid in the Pore Network of Sorbent Polymer Composite Materials on Hg Removal from Flue Gas	897
<i>Vladimiro Nikolakis, Uwe Beuscher, Michael McCutchen, Vineet Rakesh</i>	
(736e) Modeling of Biodiesel Production in Liquid-Liquid Film Reactors Including Mass Transfer Effects	898
<i>Mario Andres Noriega, Paulo C. Narvaez, Alberto Claudio Habert</i>	
(736f) Understanding Super Acidic Molten Salt Hydrate Media for Cellulose Hydrolysis	899
<i>Natalia Rodriguez Quiroz, Dionisios G. Vlachos</i>	
(736g) Probing the Reacting Interface of a Liquid-Liquid Cu-Free Sonogashira Coupling	900
<i>Benjamin Rizkin, Ryan L. Hartman</i>	
(738a) Bench-scale Measurement of Pyrolysis Products from Intact Live Fuels	901
<i>Mohammad-Saeed Safdari, Jansen Berryhill, David R. Weise, Thomas Fletcher</i>	
(738b) The Kinetic and Chemistry of Biomass Fast Pyrolysis Using Novel Micro-Sphere Micro-Reactor Technology	902
<i>Ali Zolghadr, Joseph J. Biernacki</i>	
(738c) Networks with Parallel and Sequential Reactions for Determining the Pyrolysis Kinetics of Biomass Feedstocks	903
<i>Ye Gao, Kyriacos Zygourakis</i>	
(738d) Design, Construction and Conceptual Proof of a Free Fall Fast Pyrolysis Reactor	904
<i>Diana C. Vargas, Jhoselyn Padilla, Cristina Arciniega, Kevin M. Van Geem, Daniela Almeida Streitwieser</i>	
(738e) Reaction Paths for Hemicellulose Pyrolysis Using Reactive Molecular Dynamics	905
<i>Amrutha Raghu, Phillip R. Westmoreland</i>	
(738f) Enthalpy Changes during Pyrolysis of Biomass: Interpretation of Intraparticle Gas Sampling	906
<i>Marco J. Castaldi, Simona Ciuta, Francesco Patuzzi, Marco Baratieri</i>	
(738g) Ex-Situ Catalytic Fast Pyrolysis of Beetle Killed Lodgepole Pine in Novel Ablative Reactor	907
<i>Heather Wise, Fernando Resende, Anthony Dichiaro</i>	
(744a) Aqueous Phase Reforming of Glycerol: Determining the Catalyst Support Effects	908
<i>Torrie Sewell, Rachel B. Getman, David A. Bruce</i>	
(744b) Catalytic Amino Acid Production from Biomass	909
<i>Ning Yan</i>	
(744c) Renewable Lubricant Alkanes from Biomass-Derived Platform Chemicals	910
<i>Angela M. Norton, Sibao Liu, Basudeb Saha, Dionisios G. Vlachos</i>	
(744d) Identification of Active Sites for Selective C-O Cleavage Reactions on Metals Supported on Reducible Oxides	911
<i>Lawrence Barrett, Nicholas M. Briggs, Alejandra Gomez, Valeria Herrera, Taiwo Omotoso, Steven Crossley</i>	
(744e) CO₂ Hydrogenation on Single-Site Heterogeneous Cobalt Catalyst	912
<i>Juan Jimenez, Cun Wen, Jochen Lauterbach</i>	

(744f) Coupled CO₂ Capture and Conversion to Methanol Using Solid Sorbents with a Homogeneous Catalyst	913
<i>Elizabeth A. K. Wilson, Shawn C. Eady, Trent Silbaugh, Mark Barteau, Levi T. Thompson</i>	
(744g) Selective CO₂ Hydrogenation to Methanol over Promoted Indium-Based Catalysts	914
<i>Chen-Yu Chou, Raul F. Lobo</i>	
(744h) Enhancement of Catalytic Performance of Ordered Mesoporous "One-Pot" Fe-Al₂O₃ Catalysts By Ni Incorporation in Dry Reforming of Biogas	916
<i>Karam Jabbour, Ali Saad, Lena Inati, Anne Davidson, Pascale Massiani, Nissrine El Hassan</i>	
(745a) Kinetic Evaluation of N₂ Activation in Plasma Catalytic Ammonia Synthesis	919
<i>Patrick Barboun, Prateek Mehta, Francisco Herrera, David Go, William F. Schneider, Jason C. Hicks</i>	
(745b) Atomically Dispersed Supported Metal Catalysts: Tuning Catalytic Performance with Supports and Ionic Liquid Coatings	920
<i>Melike Babucci, Chia-Yu Fang, Adam Hoffman, Alexey Boubnov, Simon R. Bare, Bruce C. Gates, Alper Uzun</i>	
(745c) Effects of Water on the Kinetics of Acetone Hydrogenation over Metal Catalysts	921
<i>Benginur Demir, Ashwin Chemburkar, Thomas Kropp, Manos Mavrikakis, Matthew Neurock, James A. Dumesic</i>	
(745d) Ab-Initio Study of the Interface between g-Al₂O₃ and Pt	922
<i>Kofi Oware Sarfo, Arielle L. Clauser, Liney Arnadottir, Melissa K Santala</i>	
(745e) Molten Salt Hydrates As Solvents in the Synthesis of Metal Oxide Catalysts	923
<i>Trang Tran, Yuanhao Yu, Justin Marlowe, George Tsilomelekis</i>	
(745f) Kinetics Investigation of Ethanol Dehydration and Dehydrogenation over a Model Oxide Catalyst	924
<i>Hussein T. Abdulrazzaq, Thomas J. Schwartz</i>	
(745g) DFT Studies of Intermetallic Gamma-Brass Structured Catalysts for Selective Hydrogenation	925
<i>Haoran He, Anish Dasgupta, Randall Meyer, Robert Rioux, Michael Janik</i>	
(745h) Correlative Structure-Bonding and Stability Studies of Pt/γ-Al₂O₃ Catalysts	926
<i>Henry Ayoola, Qing Zhu, Cecile Bonifacio, Matthew McCann, Matthew Curnan, Stephen House, Joshua Kas, John Rehr, Eric A. Stach, Wissam A. Saidi, Judith C. Yang</i>	
Author Index	