TECHNICAL PROGRAM

Chemistry in an Evolving Political Climate: Research Priorities & Career Pathways in Public Policy

Sponsored by YCC, Cosponsored by BIOL, CARB, CCPA, CEI, CELL, CEPA, CHED‡, CINF, COLL, COMSCI, CPRC, DAC, GEOC, IAC, PRES and SCHB

MONDAY EVENING

Section A

Walter E. Washington Convention Center
Halls D/E

Sci-Mix

N. L. Snyder, *Organizer*

8:00 - 10:00

27-29, 31-32, 35, 37-38, 40-42, 47-48, 53-55, 57-60. See previous listings.

TUESDAY MORNING

Section A

Grand Hyatt Washington
Constitution A

Advances in Glycan Structure & Dynamics

Host-Pathogen Interactions, Glycan-Based Vaccine Design & Glycan-Protein Interactions

Cosponsored by CELL

Financially supported by Complex Carbohydrate Research Center, JEOL

D. I. Freedberg, *Organizer*

R. J. Woods, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CARB **72.** Attachment of histo blood group antigens to human norovirus coat protein: NMR reveals unexpected complexity of the carbohydrate binding process. **T. Peters**, A. Mallagaray

9:05 CARB **73.** Beyond sweet attractions: Structural insights into host-cell glycan interactions of human pathogens. **T. Haselhorst**

9:25 CARB **74.** Investigating serotype cross-protection in carbohydrate vaccines: A molecular modelling approach. **M. Kuttel**, N. Ravenscroft

9:45 CARB **75.** Structural analysis of peptide and carbohydrate epitopes cleaved by the *Cryptococcus neoformans* catalytic monoclonal antibody 18B7. **M. Wear**, A. Bowen, R. Cordero, A. Casadevall

10:05 Intermission.

10:25 CARB **76.** Bound geometry of glycans using proteins with paramagnetic tags. **J.H. Prestegard**

10:55 CARB **77.** Protein crystallography and molecular dynamics simulations reveal an NOE-silent conformation of the GM1 glycan. **B.S. Blaum**, M. Frank, T. Stehle

11:15 CARB **78.** Molecular basis of Siglec-carbohydrate interaction. **M. Schubert**

11:35 CARB **79.** Substrate presentation and activation in neuraminidase NEU2. **O.C. Grant**, S. Makeneni, B.L. Foley, R.J. Woods

11:55 Concluding Remarks.

Understanding the Chemistry of Our Planet

Chemistry's Role in our Earth System

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CEI, CELL, CEPA, CINF, COLL, CPRC, DAC, GEOC, I&EC, INOR, ORGN, SCHB and YCC

TUESDAY AFTERNOON

Section A

Grand Hyatt Washington
Constitution A

Advances in Glycan Structure & Dynamics

Glycosaminoglycan Structure

Cosponsored by CELL

Financially supported by Complex Carbohydrate Research Center, JEOL

D. I. Freedberg, *Organizer*

R. J. Woods, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CARB **80.** Insights into the interactions between synthetic GAG and Growth Factors (FGF-1 and Midkine). M. García-Jiménez, S. Gil-Caballero, J. Muñoz-Garcia, J. de Paz, **P.M. Nieto**

2:05 CARB **81.** GAGs glycomics/interactome research using SPR. **F. Zhang**, S. Kim, J. Zhao, R.J. Linhardt

2:25 CARB **82.** Withdrawn.

2:45 Intermission.

3:05 CARB **83.** Protein-Induced changes in glycosaminoglycan dynamics: A study in pleiotrophin-glycosaminoglycan interactions. **X. Wang**

3:25 CARB **84.** Analysis of the 3D structure of fucosylated chondroitin sulfate from H. forskali and its interaction with selectins. **C. Panagos**, C. Moss, C. Bavington, B. Mulloy, T. Feizi, W. Chai, R.J. Woods, D. Uhrin

3:45 CARB **85.** Is there a structural role for 3-O-sulfation in heparan sulfate? **A. Green**, C. Larive, R. Young, L.J. Mueller

4:05 Concluding Remarks.

Understanding the Chemistry of Our Planet

Human Impacts to our Planet

Sponsored by PRES, Cosponsored by BIOL, BMGT, CARB, CEI, CELL, CEPA, CINF, COLL, CPRC, DAC, GEOC, I&EC, INOR, ORGN, SCHB and YCC

WEDNESDAY MORNING

Section A

Grand Hyatt Washington
Constitution A

Advances in Glycan Structure & Dynamics

Glycoproteins

Cosponsored by CELL

Financially supported by Complex Carbohydrate Research Center, JEOL

R. J. Woods, *Organizer*

D. I. Freedberg, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CARB **86.** Invisible glycoproteins with unusually high carbohydrate content in animal gametic cells. **K. Kitajima**

9:05 CARB **87.** Characterizing asparagine-linked glycoprotein glycans with a rapid NMR-based approach. **A.W. Barb**

9:25 CARB **88.** Unlocking the secrets of asialo-APF: Combining NMR spectroscopy and molecular dynamics to refine the complex structure-activity relationship of a (seemingly) simple antiproliferative glycopeptide. **K.M. Adams**, S.S. Mallajosyula, A.D. Mackerell, J.J. Barchi

9:45 CARB **89.** Separation of oligosaccharide and glycopeptide isomers using ion mobility-mass spectrometry. J. Hofmann, H. Hahm, H. Hinneburg, W.B. Struwe, D. Kolarich, P.H. Seeberger, **K. Pagel**

10:05 Intermission.

10:25 CARB **90.** Modeling the conformational heterogeneity of complex carbohydrates: Enhanced sampling, methods of analyses and towards a polarizable force field. **A.D. Mackerell**, M. Yang, A. Aytenfisu

10:55 CARB **91.** Routine microsecond molecular dynamics simulations of carbohydrates and glycoproteins: Prospects and limitations. **M. Frank**, R. Walker, P. Nyholm

11:15 CARB **92.** Characterization of the distinct sructural motif of α(2-8)-polysialic acid at the reducing end. **H. Azurmendi**, M. Battistel, D.I. Freedberg

11:35 Concluding Remarks.

WEDNESDAY AFTERNOON

Section A

Grand Hyatt Washington
Constitution A

Advances in Glycan Structure & Dynamics

Conformational Analysis & Less Common Approaches to Structure Determination

Cosponsored by CELL

Financially supported by Complex Carbohydrate Research Center, JEOL

R. J. Woods, *Organizer*

D. I. Freedberg, *Organizer, Presiding*

1:30 Introductory Remarks.

1:35 CARB **93.** Conformational aspects of oligosaccharides and their interactions with proteins. **G. Widmalm**

2:05 CARB **94.** Effects of exocyclic C–O bond conformation on NMR *J*-couplings in saccharides. **A.S. Serianni**

2:25 CARB **95.** NMR studies on cADPR and cADPR analogs: Conformational analysis and thermodynamics of the N/S equilibrium. **S.M. Graham**, S. Saatori

2:45 CARB **96.** Withdrawn.

3:05 CARB **97.** NMR methodology for OH/OH hydrogen bond detection: Diols, networks, and stereochemical assignments. **D.J. O'Leary**

3:25 Intermission.

3:45 CARB **98.** Mannosylated surfaces exhibit self-adhesive and water-structuring properties; model for pathogen surface. **K. Perera**, P. Chandran

4:15 CARB **99.** Atomic-level structure characterization of carbohydrate pre and post lignin treatment by dynamic nuclear polarization: Enhanced solid state NMR. **H. Luo**

4:35 CARB **100.** Simple methods for *de novo* structural determination of glucose-containing underivatized oligosaccharides. **C.K. Ni**

4:55 Concluding Remarks.

CATL

Division of Catalysis Science and Technology

K. Ramasamy, *Program Chair*

OTHER SYMPOSIA OF INTEREST:

Energy & Fuels Storch Award in Fuel Science: Symposium in Honor of Umit S. Ozkan (see *ENFL*, Sun, Mon)

5th International Symposium on Mesoporous Zeolites (see *ENFL*, Wed)

Advanced Nanomaterials Catalysts for Sustainable Energy & Fuels (see *ENFL*, Sun, Mon, Tue)

Green Chemistry & the Environment (see *ENVR*, Wed)

Environmental Applications of Liquid-Phase Catalysis for Green Chemical Processes of Renewable Materials (see *ENVR*, Sun, Mon, Wed)

Nano-Enabled Water Treatment Technologies: Applications & Implications (see *ENVR*, Mon, Tue, Wed)

BUSINESS MEETINGS:

CATL Business Meeting, 5:30 PM: Mon

SUNDAY MORNING

Section A

Walter E. Washington Convention Center
Room 101

Catalytic Transformation of Renewable Plant Biomass to Enhance Global Economy

Cosponsored by ENFL

N. Yan, X. Zhang, *Organizers*, *Presiding*

9:00 CATL **1.** Nano copper-nickel alloy catalysts for selective hydrothermal conversion of oleic acid into heptadecane with methanol. **J. Fu**, Z. Zhang, Q. Yang, X. Lu

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

‡ *Cooperative Cosponsorship*

9:20 CATL **2.** Selective conversion of cellulose into C2-C4 alcohols on solid catalysts. **H. Liu**

9:50 CATL **3.** Photocatalytic cleavage of lignin into aromatics. **F. Wang**, N. Luo, T. Hou

10:20 CATL **4.** Conversion of bark to bio-based polyols via liquefaction and alkoxylation reactions. **N. Yan**

10:50 Intermission.

11:05 CATL **5.** Biphasic tandem catalytic process for renewable fuel production. **H. Lin**

11:25 CATL **6.** Effect of metal properties on glycerol hydrogenolysis over platinum and ruthenium catalysts. **W. Zhou**, Z. Yujun, Y. Wang, S. Wang, X. Ma

11:45 CATL **7.** High efficiency production of acrylates from lactic acid. **T.R. Eaton**, N.A. Rorrer, V. Sanchez i Nogue, K. Meek, L. Manker, D. Brandner, M. Biddy, E. Karp, G. Beckham

12:05 CATL **8.** Catalyst and process development for the hydroprocessing of fast pyrolysis bio-oil. **M.V. Olarte**, H. Wang, D. Santosa, J. Frye, P. Meyer, S. Lee, S.B. Jones, C. Drennan, J.S. Choi, A. Zacher

Section B

Walter E. Washington Convention Center
Room 102B

Mixed Metal Oxide Catalysis

C. Alvarez-Vasco, R. Fushimi, D. Shekhawat, *Organizers*

K. K. Ramasamy, I. E. Wachs, *Organizers*, *Presiding*

8:30 CATL **9.** Transesterification of glycerol and dimethyl carbonate to glycerol carbonate over mixed metal oxide catalysts. **L. Yajin**, D. He

8:50 CATL **10.** Silica support early transition metal catalysts: Spectroscopic characterization, trends in coordination environment, speciation on the surface and effects on reactivity. N. Peek, S. Klepper, D. Jeffcoat, S.L. Scott, **A.E. Stiegman**

9:10 CATL **11.** Developing perovskite materials for oxidation reactions. **J.W. Lekse**, S. Natesakhawat, Y. Zhou, D. Tafen, D. Alfonso, C. Gounaris, C. Hanselman, C. Matranga, D. Kauffman, J. Lee

9:30 CATL **12.** Understanding of mixed metal oxide anionic clays as solid base catalysts for biofuels production. **S.K. Beaumont**

9:50 CATL **13.** Multi-spectral photocatalysis for improved degradation of recalcitrant contaminants from aqueous systems. **E. Asenath-Smith**, E. Ambrogi, J. Brame

10:10 Intermission.

10:25 CATL **14.** Role of surface and bulk structures of perovskites in catalyzing acid-base reactions. G. Foo, F. Polo Garzon, V. Fung, D. Jiang, **Z. Wu**

10:55 CATL **15.** *Operando* spectroscopy during ethylene polymerization by supported CrO_x/SiO_2 catalysts: Role of promoters. **A. Chakrabarti**, I.E. Wachs

11:15 CATL **16.** Cyclodehydration of 1,4-butanediol to tetrahydrofuran over Zr-Al mixed oxide catalysts. **K.T. Li**, K. Chen

11:35 CATL **17.** Monitoring the adsorption and decomposition of dimethyl methylphosphonate on mesoporous metal oxides. **S.M. Holdren**, K. Huynh, J. Hu, W. Gibbons, B.W. Eichhorn, M.R. Zachariah

11:55 CATL **18.** Stabilizing effects of polyoxoniobates on molecular copper-oxo species in alkaline water for water oxidation catalysis. **Q. Yin**, Y. Hu, E.N. Glass, S.M. Lauinger, M.D. Nyman, C.L. Hill

Section C

Walter E. Washington Convention Center
Room 102A

Metal-Support Interactions in Catalysis: Modeling, Characterization & Design

A. Bruix, T. Duchon, S. D. Senanayake, *Organizers*

A. Baber, *Presiding*

8:30 CATL **19.** CO oxidation at the interface between FeO and nobel metals: Interface and size effects. **F. Yang**

9:05 CATL **20.** Reactivity of O_2 with single-site, low-valent vanadium in metal-organic chains at surfaces. **T. Morris**, C.D. Tempas, D. Wisman, B.J. Cook, A.V. Polezhaev, K.G. Caulton, S.L. Tait

9:25 CATL **21.** Atomic-scale insight into single atom catalysis. **A. Therrien**, E.H. Sykes, J. McEwen

10:00 Intermission.

10:15 CATL **22.** Au nanoparticle interactions with TiO_2(110) and their modification of the reactivity. **G. Thornton**

10:50 CATL **23.** Au-TiO_2 interfaces in the catalysis of low-temperature oxidation and H_2 photoproduction from water. **F. Zaera**

11:25 CATL **24.** Theoretical insights on CO oxidation over Au/TiO2: A comprehensive picture of active sites, catalysts deactivation and moisture effects. **Z. Duan**, G. Henkelman

11:45 CATL **25.** Supported metal nanoparticle catalysts: Predicting how size and support effect metal atom energetics and thus catalytic performance. **C.T. Campbell**, Z. Mao

Section D

Walter E. Washington Convention Center
Room 103B

Cooperative Catalysis at Surfaces & Interfaces: Impact on Chemistry & Energy Frontiers

Electrocatalysis

Cosponsored by ENFL

M. Cargnello, Z. Wu, *Organizers*

S. Zhang, *Organizer, Presiding*

M. Cargnello, *Presiding*

8:30 Introductory Remarks.

8:35 CATL **26.** Reaction mechanisms in heterogeneous catalysis and electrocatalysis involving cooperation between different sites from quantum mechanics. **W.A. Goddard**

9:05 CATL **27.** Controlling metal nanoparticle interactions with nanoscale-supports to enhance nanoparticle catalysis for selective CO_2 reduction. **S. Sun**

9:35 CATL **28.** In Situ insight on CO_2 activation on Cu(111) surfaces with subsurface oxide: Fundamental understanding on the first step of CO_2 reduction reaction by APXPS and DFT. **C. Zhang**, M. Favaro, H. Xiao, T. Cheng, W.A. Goddard, J. Yano, E. Crumlin

9:55 Intermission.

10:10 CATL **29.** Energy and fuels from tailored nanomaterials and electrochemical interfaces. E. Coleman, D. Li, H. Lv, R. Wang, D. Strmcnik, P. Lopes, N. Markovic, **V. Stamenkovic**

10:40 CATL **30.** Core-Shell nanostructures in electrocatalysis. L. Wang, **C. Wang**

11:10 CATL **31.** Electrocatalytic reduction of CO_2 by metal/ionic liquid interfaces: Theoretical insights. **S. Winikoff**, M. Neurock

11:30 CATL **32.** Strong metal-oxide and metal-phosphide interactions for enhanced electrocatalysis. **H. Wang**

12:00 CATL **33.** Spatially separated dual cocatalysts supported on semiconductor prepared by atomic layer deposition for efficient photocatalytic hydrogen production. J. Zhang, **C. Chaoqiu**, Z. Gao, Y. Qin

Section E

Walter E. Washington Convention Center
Room 140A

Advanced Electrocatalysis for Energy Conversion & Storage

Oxygen Reduction

N. Danilovic, A. B. Padmaperuma, C. Wang, B. Xu, *Organizers*

A. Holewinski, *Organizer, Presiding*

C. Wang, *Presiding*

8:30 CATL **34.** Advancing PGM-free fuel cell catalysts through the ElectroCat (Electrocatalysis) consortium. **S.T. Thompson**, A.R. Wilson, D. Papageorgopoulos

8:50 CATL **35.** Determining the role of the metal in non-precious metal catalysts for the oxygen reduction reaction. **J. Varnell**, C. Tse, A.A. Gewirth

9:10 CATL **36.** Analysis of the mechanism of electrochemical oxygen reduction and development of alloy catalysts for low temperature fuel cells. **S. Linic**

9:50 Intermission.

10:10 CATL **37.** Electrochemical interfaces, electrocatalysis and green energy. P. Lopes, D. Strmcnik, V. Stamenkovic, **N. Markovic**

10:50 CATL **38.** Perflourinated alkylamine modified Pt nanoparticles as hyperactive ORR electrocatalyst for fuel cell application. **P. Joshi**, M. Miyake, K. Miyabayashi

11:10 CATL **39.** Enabling sustainable non noble metal electrocatalysts for oxygen reduction reaction. **S. Mukerjee**, Q. Jia

11:50 CATL **40.** Withdrawn.

Section F

Walter E. Washington Convention Center
Room 140B

Catalysis at the Sub-Nanometer Scale

Activity of Highly Dispersed Catalysts

H. Xin, *Organizer*

A. M. Karim, *Organizer, Presiding*

8:30 CATL **41.** Ligand–free sub–nanometer metal clusters for catalysis in organic synthesis. **A. Leyva-Perez**, A. Corma, M.A. Rivero-Crespo, M. Tejeda-Serrano

8:55 CATL **42.** Tailoring mesoporous silica nanoparticles for robust immobilization of lipase and biocatalysis. **M. Kalantari**

9:15 CATL **43.** *In-situ* surface/bulk spectroscopic and kinetic investigations of alcohol conversions over metal oxide catalysts. **S. Tan**, Y. Cheng, L. Daemen, D. Lee, H. Lee, Y. Ma, B. Doughty, D.A. Lutterman

9:40 CATL **44.** Infrared spectroscopic studies of propene and propene oxide uptake, binding, and reactivity on TiO_2-SiO_2 binary catalysts. **D.M. Driscoll**, N.S. Sapienza, J.R. Morris

10:00 Intermission.

10:20 CATL **45.** Conversion of CO_2 into useful fuels using Cu_x/TiO_2 photocatalysts. **N.A. Deskins**, S. Iyemperumal

10:45 CATL **46.** Methanol synthesis from CO_2 over size-selected sub-nanometer copper catalyst: Cluster size vs charge transfer. **B. Yang**, C. Liu, A. Halder, E. Tyo, S. Seifert, P. Zapol, L.A. Curtiss, S. Vajda

11:10 CATL **47.** Pt-Ni nanoscale catalysts synthesized by atomic layer deposition for complete reduction of C=C and C=O bonds in oleic acid without using H_2 and a solvent. **J. Fu**, H. Chen, X. Lu

Electrochemical Technologies for Water Purification

Sponsored by ENVR, Cosponsored by CATL and CEI

Energy & Fuels Storch Award in Fuel Science: Symposium in honor of Umit S. Ozkan

Sponsored by ENFL, Cosponsored by CATL

SUNDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 101

Catalytic Transformation of Renewable Plant Biomass to Enhance Global Economy

Cosponsored by ENFL

N. Yan, X. Zhang, *Organizers*, *Presiding*

1:30 CATL **48.** What is lignin recalcitrance? A critical analysis of lignins derived from mechanocatalytic biorefining and organosolv process. **R. Rinaldi**

2:00 CATL **49.** Selective production of arenes via direct lignin upgrading over a niobium-based catalyst. **Y. Wang**, Y. Shao, S. Yang, Y. Cheng

2:30 CATL **50.** Mechanochemical synthesis of nanocatalysts for biomass conversion. **R. Luque**

3:00 CATL **51.** Microwaves and catalysis for the fast and selective valorisation of biomass: From hydrolysis to oxidation and hydrogenation reactions. **J.A. Lopez-Sanchez**

3:30 Intermission.

3:45 CATL **52.** Continuous catalytic production of deoxygenated hydrocarbon fuels from biomass pyrolysis oil. **J. Ha**

4:15 CATL **53.** Hydrotreating of in situ catalytic fast pyrolysis bio-oil. **H. Wang**, D. Santosa, F.A. Agblevor

4:35 CATL **54.** Valorization of nanoscale lignin extracted from agricultural biomass by deep eutectic solvents (DES). **R. Lou**, X. Zhang

4:55 CATL **55.** Stability of heterogeneous heteropolyacids for muconic acid upgrading. **A. Settle**, J.H. Cooper, L. Berstis, K. Kinley, H. Hu, G. Beckham, R.M. Richards, D. Vardon

Section B

Walter E. Washington Convention Center
Room 102B

Mixed Metal Oxide Catalysis

C. Alvarez-Vasco, K. K. Ramasamy, I. E. Wachs, *Organizers*

R. Fushimi, D. Shekhawat, *Organizers*, *Presiding*

1:30 CATL **56.** Tuning the electrochemical activity of layered nickleate oxides for oxygen reduction: Effect of surface termination and composition. **E. Nikolla**

2:00 CATL **57.** Understanding and controlling the activity and stability of Pd/Pt oxide catalysts for methane activation. **M. Cargnello**, E. Goodman, A. Yang, S. Dai, C. Wrasman, S. Bare, A. Hoffman, G. Graham, X. Pan

2:30 CATL **58.** $CeO_x/TiO_2(110)$ and $RuO_x/TiO_2(110)$ as active systems for CO oxidation, the water-gas shift and CO_2 hydrogenation reactions. **J. Rodriguez**

2:50 CATL **59.** Syntheses of high yield MMO catalyst for direct propane oxidation to acrylic acid. **J. Xu**, L. Bogan

3:10 Intermission.

3:25 CATL **60.** Olefin metathesis by supported MoO_x/Al_2O_3 catalysts. **A. Chakrabarti**, I.E. Wachs

3:45 CATL **61.** Catalytic dehydrogenative coupling of amines. **D. Ainembabazi**, N. Tiedemann, A. Voutchkova

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

4:05 CATL **62.** Introducing trace potassium as the electronic and structural modifier to enhance the oxidation of Co_3O_4 catalyst. C. Wang, W. Wang, **W. Li**, Y. Guo, Y. Guo, G. Lu

4:25 CATL **63.** One pot green syntheses of $CuO\text{-}Cu_2O/g\text{-}C_3N_4$ nanosheets for enhanced catalysis of nitroarenes. **T. Aditya**, T. Pal

Section C

Walter E. Washington Convention Center
Room 102A

Metal-Support Interactions in Catalysis: Modeling, Characterization & Design

T. Duchon, S. D. Senanayake, *Organizers*

A. Bruix, *Organizer, Presiding*

1:30 CATL **64.** Fluxionality and statistical ensemble nature of surface-supported cluster catalysts. **A. Alexandrova**

2:05 CATL **65.** Identifying the active site of the water-gas shift reaction over platinum based catalysts. **A. Heyden**, E. Walker, S. Ammal

2:40 CATL **66.** Computational modeling of catalytic metal/metal-oxide nanostructures. **K. Neyman**

3:15 Intermission.

3:30 CATL **67.** Adsorption energy correlations at the metal-support boundary. **P. Mehta**, J.P. Greeley, W. Delgass, W.F. Schneider

3:50 CATL **68.** Hydrogenation of CO_2 to C1 (CO, CH_4, CH_3OH) molecules on oxide-supported catalysts. **S. Kattel**, J.G. Chen, P. Liu

4:25 CATL **69.** Study of the interface between Al_2O_3 and Pt (111) by DFT calculations and high-resolution TEM. **K. Oware Sarfo**, A.L. Clauser, Z.D. McClure, M. Santala, L. Arnadottir

4:45 CATL **70.** Metal-ceria interactions and the catalytic activity for hydrogen production and methane dry reforming: A theoretical perspective. **M. Ganduglia-Pirovano**, P. Lustemberg, J. Carey, M. Nolan

Section D

Walter E. Washington Convention Center
Room 103B

Cooperative Catalysis at Surfaces & Interfaces: Impact on Chemistry & Energy Frontiers

Photocatalysis & Oxide Catalysis

Cosponsored by ENFL

M. Cargnello, *Organizer*

Z. Wu, S. Zhang, *Organizers*, *Presiding*

1:30 CATL **71.** Coupling solar energy into catalytic organic synthesis. **Y. Xiong**

2:00 CATL **72.** Quantification of acid site densities on zeolites in the presence of solvents via determination of extinction coefficients of adsorbed pyridine. **N. Gould**, B. Xu

2:20 CATL **73.** Beautiful surface chemistry behind efficient catalysis. **W. Huang**

2:50 CATL **74.** Cooperative defect/surface mechanism in deoxygenation reactions over reducible metal oxides. **X. Xiao**, B. Johnson, H. Bergstrom, C. Hargus, A. Peterson

3:10 Intermission.

3:20 CATL **75.** Bifunctional strategy coupling Y_2O_3 catalyzed alkanal decomposition with methanol-to-olefins catalysis for enhanced lifetime. **A. Bhan**

3:50 CATL **76.** Kinetics and mechanism of methanol conversion over anatase titania nanoshapes. **G. Foo**, G. Hu, Z.D. Hood, M. Li, D. Jiang, Z. Wu

4:10 CATL **77.** Fundamental studies on CO_2 hydrogenation and the low-temperature water-gas shift reaction on metal-carbide interfaces. **J. Rodriguez**

4:40 CATL **78.** Support effect in oxide catalysis: Methanol oxidation on vanadia/ceria. **T. Kropp**, J.A. Paier, J. Sauer

5:00 CATL **79.** Cooperativity between acid-base and redox sites on metal oxide surfaces. **D.R. Mullins**

Section E

Walter E. Washington Convention Center
Room 140A

Advanced Electrocatalysis for Energy Conversion & Storage

Oxygen Reduction & Evolution

A. B. Padmaperuma, C. Wang, B. Xu, *Organizers*

A. Holewinski, *Organizer, Presiding*

N. Danilovic, *Presiding*

1:30 CATL **80.** Development of electrocatalysts for energy technologies. **G.L. Soloveichik**

2:10 CATL **81.** Withdrawn.

2:30 CATL **82.** Iridium on Steroids: using rigid, polycyclic, aliphatic molecules as non-conductive linkers to bind catalytic centers to metal oxide semi-conductors. **A. Bloomfield**, S. Chaudhuri, S. Hedstrom, V.S. Batista, R.H. Crabtree

2:50 Intermission.

3:10 CATL **83.** Understanding the active sites and reaction mechanism for oxygen electrocatalysis on ruthenium dioxide surfaces. **R. Rao**, Y. Shao-Horn

3:50 CATL **84.** Exceptional electrocatalytic oxygen evolution via tunable charge transfer interactions in Ruddlesden-Popper oxides. **R.P. Forslund**, K.P. Johnston, A.M. Abakumov, A.M. Kolpak, K.J. Stevenson

4:10 CATL **85.** Water oxidation in strong acid using cobalt-based POMs as catalysts. **M. Tao**, Q. Yin, C.L. Hill

4:30 CATL **86.** Towards a solar fuels future: Theoretical metrics for photoelectrocatalyst screening. **J. Montoya**, A. Singh, S. Dwaraknath, K. Persson

Section F

Walter E. Washington Convention Center
Room 140B

Catalysis at the Sub-Nanometer Scale

Synthesis, Characterization & Mechanisms

A. M. Karim, *Organizer*

H. Xin, *Organizer, Presiding*

1:30 CATL **87.** Highly efficient oxygen reduction electrocatalyst derived from electrospun interconnected Co-N/C nanofiber networks. **N. Wenjun**

1:50 CATL **88.** Electrochemical oxygen reduction by atomically dispersed Pt on sulfur-doped zeolite-templated carbons: Selective production of H_2O_2 instead of H_2O. **M. Choi**, H. Kim, C. Choi

2:15 CATL **89.** Influence of phosphine substitution on the synthesis and properties of gold clusters. **G.E. Johnson**, J. Laskin, U. Reveles, M. Ligare

2:45 CATL **90.** Machine learning guided interpretation of X-ray absorption data for ultradispersed catalysts. **J. Timoshenko**, D. Lu, S. Yoo, A. Frenkel

3:10 Intermission.

3:30 CATL **91.** Spectroscopic signatures and reactivity of CO adsorbed to Pt atoms, Pt oxide clusters, and metallic Pt clusters on anatase TiO_2. **P. Christopher**

4:10 CATL **92.** Insights from global optimization and ab initio thermodynamics on inverse catalysts: The case of Cu-supported ZnO clusters. T. Reichenbach, M. Walter, M. Moseler, B. Hammer, **A. Bruix**

4:35 CATL **93.** Density-functional modeling of materials for single-atom catalysis based on nanostructured ceria. **K. Neyman**

Electrochemical Technologies for Water Purification

Sponsored by ENVR, Cosponsored by CATL and CEI

Energy & Fuels Storch Award in Fuel Science: Symposium in honor of Umit S. Ozkan

Sponsored by ENFL, Cosponsored by CATL

Environmental Applications of Liquid Phase Catalysis for Green Chemical Processes of Renewable Materials

Sponsored by ENVR, Cosponsored by CATL and ENFL

MONDAY MORNING

Section A

Walter E. Washington Convention Center
Room 101

Catalytic Transformation of Renewable Plant Biomass to Enhance Global Economy

Cosponsored by ENFL

N. Yan, X. Zhang, *Organizers*, *Presiding*

8:30 CATL **94.** Recalcitrance: The plant cell wall and cellulosic biofuels. **A.J. Ragauskas**

9:00 CATL **95.** Depolymerization of cellulose by carbon catalysts. **A. Fukuoka**

9:30 CATL **96.** Stabilization with aldehydes for the high yield production of targeted monomer mixtures from lignin during integrated biomass depolymerization. **J. Luterbacher**

10:00 CATL **97.** Catalytic conversion of glucose and industrial-grade sugars derived from corn and wood into 5-HMF in a biphasic continuous-flow tubular reactor. **C.C. Xu**

10:30 Intermission.

10:45 CATL **98.** Catalytic conversion of bioethanol to 1,3-butadiene using bifunctional catalysts: The role of active sites via in situ spectroscopy. W. Taifan, **J. Baltrusaitis**

‡ *Cooperative Cosponsorship*

11:05 CATL **99.** Guerbet ethanol coupling over a stable Cu-MgO-Al_2O_3 catalyst. **K.K. Ramasamy**, M. Gray, M. Guo

11:25 CATL **100.** Chemocatalytic production of ethanol from lignocellulose via methyl glycolate. **A. Wang**

11:45 CATL **101.** Catalytic conversion of bioderived muconic acid to produce adipic acid and dimethyl terephthalate. **D. Vardon**, A. Settle, L. Berstis, S. Christensen, N. Cleveland, K. Kinley, J. Cooper, H. Hu, M.F. Crowley, R.M. Richards, G. Beckham

Section B

Walter E. Washington Convention Center Room 102B

Mixed Metal Oxide Catalysis

K. K. Ramasamy, I. E. Wachs, Organizers

C. Alvarez-Vasco, R. Fushimi, D. Shekhawat, *Organizers*, *Presiding*

8:30 CATL **102.** Understanding elemental steps in conversion of alcohols and diols on model early transition metal oxide catalysts. **Z. Dohnalek**

9:00 CATL **103.** Uniform sites in dispersed metal oxide catalysts for olefin polymerization, metathesis, and oxidation. **S.L. Scott**

9:30 CATL **104.** In situ Raman spectroscopic analysis during coal oxidation over hematite and taconite in the chemical looping process. **D. Miller**, M.W. Smith, D. Shekhawat

9:50 CATL **105.** Effect of dopants in the support of copper-ceria catalysts on the performance for preferential CO oxidation in H_2-rich stream. **J. Oh**, J. Bae

10:10 Intermission.

10:25 CATL **106.** Heterojunction of TiO_2 nanoparticle embedded into ZSM-5 to layer-structured MoS_2 fabricated by pulsed laser ablation and microwave technique in deionized water: Application in drinking water purification. **A. Balati**, H.J. Shipley, K. Nash

10:45 CATL **107.** Oxidative dehydrogenation at $MoVO_x$ materials: Understanding the electronic structure from various DFT approaches. T. Fjermestad, W. Li, G. Rugg, **A. Genest**, N. Roesch

11:05 CATL **108.** Ternary oxide semiconductor nanostructures for photoelectrochemistry and photocatalysis. A. Varga, G.F. Samu, K. Rajeshwar, **C. Janaky**

11:25 CATL **109.** Routes to ternary molybdenum oxide catalysts based on bimetallic complexes. **A.W. Apblett**, A.M. Moneeb, A. Bagabas, A. Alabdulrahman

11:45 CATL **110.** Computational studies on the surface structure and reactivity of mixed metal oxide catalysts: VO_x/TiO_2, SrO_x/La_2O_3, and PdO_x/Co_3O_4 for CH_3OH and CH_4 oxidation. **S. Li**, S. Wang, N. Li, L. Cong, C. Zhao

Section C

Walter E. Washington Convention Center Room 102A

Metal-Support Interactions in Catalysis: Modeling, Characterization & Design

A. Bruix, T. Duchon, *Organizers*

S. D. Senanayake, *Organizer, Presiding*

8:30 CATL **111.** Manganese promotion of rhodium-based nanocatalysts. **P.C. Carrillo**, M.G. White

8:50 CATL **112.** ^{18}O and ^{16}O oxygen exchange on model Rh/CeO_x and Rh/CeOxFy systems. **M. Kettner**, T. Duchon, P. Kus, V. Nehasil

9:10 CATL **113.** Adsorbate-mediated strong metal-support interactions in supported Rh catalysts. **P. Christopher**

9:45 CATL **114.** Low-temperature methane combustion over Pd/H-ZSM-5: Chemical state of Pd modulated by acidic sites of H-ZSM-5. **Y. Guo**, J. Ma, Y. Lou, W. Wang, H. Zhao, W. Hu, W. Li, W. Zhan, Y. Guo, P. Hu, G. Lu

10:20 Intermission.

10:35 CATL **115.** Hierarchical catalyst design based on metal-support interactions. **I.I. Slowing**

11:10 CATL **116.** Impact of interfacial charge transfer on the performance of Pd/C catalysts. **R.G. Rao**, R. Blume, T. Hansen, E. Fuentes, K. Dreyer, D. Hibbitts, Y.J. Chabal, R. Schloegl, J. Tessonnier

11:30 CATL **117.** Nanocatalysts for Syngas conversion to higher hydrocarbons using Si-microreactor. T.L. Davis, R. Abrokwah, T. Hossain, N. Mohammad, V.G. Deshmane, S. Woosley, S. Aravamudhan, D. Mainardi, **D. Kuila**

11:50 CATL **118.** Metal-ligand complexation through redox assembly at surfaces characterized by vibrational spectroscopy. **C.G. Williams**, M. Wang, D. Skomski, C. Tempas, L.L. Kesmodel, S.L. Tait

Section D

Walter E. Washington Convention Center Room 103B

Cooperative Catalysis at Surfaces & Interfaces: Impact on Chemistry & Energy Frontiers

Oxide Catalysis

Cosponsored by ENFL

M. Cargnello, S. Zhang, *Organizers*

Z. Wu, *Organizer, Presiding*

M. Cargnello, *Presiding*

8:30 CATL **119.** Activation of the carbon-hydrogen bond by oxides and halides. **H. Metiu**, S. Chrétien, H. Kristoffersen

9:00 CATL **120.** Cooperative catalysis at solid-liquid interfaces of non-innocent supports. **I.I. Slowing**

9:20 CATL **121.** Single facet nano-shaped materials as model catalysts for alcohol conversion. **Y. Wang**

9:50 CATL **122.** K_2O/WO_x/Al_2O_3 catalyst structure for sour natural gas treatment. B. Li, M. Zhu, J. Jehng, I.E. Wachs, Z. Wu, **J. Baltrusaitis**

10:20 Intermission.

10:35 CATL **123.** Metal-support cooperativity in dispersed Re catalysts for olefin metathesis. **S.L. Scott**

11:05 CATL **124.** Role of Lewis and Brønsted acid sites of alumina in the activation of methyltrioxorhenium (MTO) for olefin metathesis. **F. Zhang**, K.C. Szeto, L. Delevoye, R. Gauvin, M. Taoufik, S.L. Scott

11:25 CATL **125.** Selectivity control of acid-base reaction via surface reconstruction of perovskite catalysts. **F. Polo Garzon**, S. Yang, V. Fung, G. Foo, E.E. Bickel, M.F. Chisholm, D. Jiang, Z. Wu

11:45 CATL **126.** Cooperativity between nanoparticles and supports for sintering-resistance catalysts through nanostructured materials. **S. Dai**

Section E

Walter E. Washington Convention Center Room 140A

Advanced Electrocatalysis for Energy Conversion & Storage

CO_2 Reduction & Hydrogen Evolution

A. Holewinski, A. B. Padmaperuma, C. Wang, *Organizers*

B. Xu, *Organizer, Presiding*

C. Wang, *Presiding*

8:30 CATL **127.** Proton reduction using hydrogenase-modified silicon photoelectrodes. **N.C. Anderson**, N.R. Neale, P.W. King

8:50 CATL **128.** Giant core/shell quantum dots for efficient and stable photoelectrochemical solar hydrogen production. **R. Adhikari**, K. Basu, Y. Zhou, F. Vetrone, D. Ma, S. Sun, F. Vidal, H. Zhao, F. Rosei

9:10 CATL **129.** Water splitting and the making of renewable chemicals. **I. Chorkendorff**

9:50 Intermission.

10:10 CATL **130.** Factors affecting the activity and selectivity of Cu for the electrochemical reduction of CO_2. **A.T. Bell**

10:50 CATL **131.** Effect of the interlayer spacing and charge of 1T-MoS_2 on the electrocatalytic activity for the hydrogen evolution reaction. **N.H. Attanayake**, A.C. Thenuwara, A. Patra, Y. Aulin, H. Chakraborty, E. Borguet, M.L. Klein, J.P. Perdew, D.R. Strongin

11:10 CATL **132.** Electrocatalysts for efficient and selective reduction of CO_2 to ethylene. **P.J. Kenis**, S. Verma, A.A. Gewirth

11:50 CATL **133.** Highly dense Cu nanowires for electrochemical conversion of CO_2. **D. Raciti**, C. Wang

Section F

Walter E. Washington Convention Center Room 140B

2017 ACS Catalysis Lectureship for the Advancement of Catalytic Science

V. A. Schmidt, *Organizer*

D. J. Mindiola, *Organizer, Presiding*

8:00 Introductory Remarks.

8:10 CATL **134.** Establishing trends in actinide bonding using redox-active ligands. **S.C. Bart**, S.A. Pattenaude, S.S. Galley, T.E. Albrecht-Schmitt

8:35 CATL **135.** Catalytic reactions in complex molecular environments. **S.J. Miller**

9:00 CATL **136.** New strategies for catalytic C-H activation via metal-oxo and metal-hydroxo intermediates. **J.T. Groves**

9:25 Intermission.

9:40 CATL **137.** Innovation at Merck Process R&D via discovery and development of new catalytic reactions. **R. Ruck**

10:05 CATL **138.** Electrocatalytic ammonia splitting at ambient temperatures. **M.R. Smith**

10:30 CATL **139.** Radical-type reactivity derived from redox non-innocence in the (dadi)Ti(L/X) system. **P.T. Wolczanski**, S.P. Hines, S.N. MacMillan, T. Cundari

10:55 CATL **140.** Photosensitization of organometallic catalysis: Switching on new reactions of value to medicinal and process chemists. **D.W. MacMillan**

11:20 CATL **141.** Catalysis with earth abundant transition metals: The interplay of electronic structure and applications. **P.J. Chirik**

Energy & Fuels Storch Award in Fuel Science: Symposium in honor of Umit S. Ozkan

Sponsored by ENFL, Cosponsored by CATL

Environmental Applications of Liquid Phase Catalysis for Green Chemical Processes of Renewable Materials

Sponsored by ENVR, Cosponsored by CATL and ENFL

MONDAY AFTERNOON

Section A

Walter E. Washington Convention Center Room 101

Advances in Computational Catalysis

G. Mpourmpakis, R. Surendran Assary, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 CATL **142.** In silico prediction of materials for energy applications. **D.G. Vlachos**

1:35 CATL **143.** Improving catalysts by unearthing the reactions that hinder catalysis. **P.M. Zimmerman**

2:05 CATL **144.** Computational design of advanced nanoalloy materials for catalysis and beyond. **K. Neyman**

2:35 Intermission.

2:50 CATL **145.** Kinetic modeling of dual-site catalysts: Limitations and prospects. **M.J. Janik**

3:20 CATL **146.** Computational catalysis in complex environments. **K. Johnson**, L. Li, J. Ye, N. Vo, A. Bahusetty, D. Lambrecht

3:50 CATL **147.** Insights into Pd-catalyzed aerobic alcohol oxidation via first-principles microkinetic analysis. **J.R. Schmidt**

4:10 Concluding Remarks.

TECHNICAL PROGRAM

Section B

Walter E. Washington Convention Center
Room 102B

Emerging Catalytic Processes for Methane Conversion

Cosponsored by ENFL

D. Liu, *Organizer*

E. Hensen, Y. Lei, *Organizers*, *Presiding*

X. Bao, D. Liu, *Presiding*

1:00 CATL **148.** How do Ru and Ni surfaces catalyze methane decomposition? New insights for catalyst design. **R.L. Arevalo**, S.M. Aspera, M.S. Escano, H. Nakanishi, H. Kasai

1:20 CATL **149.** Catalytic transformation of methane to acetic acid under mild conditions. **F. Tao**

1:50 CATL **150.** Partial oxidation of methane to oxygenates using bi- and trimetallic Au/Pd/Cu catalysts. M. Ab Rahim, **R.D. Armstrong**, S. Freakley, S. Taylor, G. Hutchings

2:20 CATL **151.** Direct conversion of natural gas to products: Challenges and opportunities for the field of catalysis. **A.T. Bell**

2:55 Intermission.

3:10 CATL **152.** Simplicity and the complexity of the direct methane to methanol conversion. **J. van Bokhoven**

3:45 CATL **153.** Tailoring conversion and selectivity of non-oxidative activation of methane via hydrogen-permeable tubular membrane reactor. **D. Liu**, M. Sakbodin, E.D. Wachsman

4:15 CATL **154.** Selective oxidation of methane to methanol in zeolites: A window of opportunity. **A. Kulkarni**

Section C

Walter E. Washington Convention Center
Room 102A

Metal-Support Interactions in Catalysis: Modeling, Characterization & Design

A. Bruix, T. Duchon, S. D. Senanayake, *Organizers*

S. Jatib Khatib, *Presiding*

1:30 CATL **155.** Growth and surface chemistry of IrO_2. Z. Liang, T. Li, M. Kim, R. Rai, A.R. Asthagiri, **J.F. Weaver**

2:05 CATL **156.** Comparison of growth and sintering of monometallic and bimetallic nanoparticles over reducible CeO_2(111) thin films: Effect of metal-support interactions. **J. Zhou**

2:40 CATL **157.** Catalysis at multiple length scales: Crotonaldehyde hydrogenation at nanoscale and mesoscale interfaces in platinum–cerium oxide catalysts. **L. Baker**, Y. Mueanngern, X. Yang, Y. Tang, F. Tao

3:15 Intermission.

3:30 CATL **158.** Confined nanocatalysts in nanotubes produced by atomic layer deposition. **Y. Qin**, Z. Gao, B. Zhang, C. Chen

3:50 CATL **159.** Acetaldehyde from Bioethanol oxidation: Describing synergy between metal and supports (ZrO_2 and CeO_2). **P.H. Rana**

4:10 CATL **160.** Electronic metal-support interactions and the production of hydrogen through the water-gas shift and the reforming of alcohols or methane. **J. Rodriguez**

4:45 CATL **161.** Orientation-dependent redox properties of ceria–copper interface. **T. Duchon**, J. Höcker, J. Hackl, M. Aulicka, K. Veltruska, V. Matolin, J. Falta, S. Nemsak, C.M. Schneider, J. Flege

Section D

Walter E. Washington Convention Center
Room 103B

Cooperative Catalysis at Surfaces & Interfaces: Impact on Chemistry & Energy Frontiers

Metal Catalysis

Cosponsored by ENFL

M. Cargnello, S. Zhang, *Organizers*

Z. Wu, *Organizer, Presiding*

M. Cargnello, *Presiding*

1:30 CATL **162.** Amine-modified silicates as acid/base bifunctional catalysts and catalyst supports. **C.W. Jones**

2:00 CATL **163.** Investigation of Pd-Ceria catalysts for selective hydrogenation of acetylene in ethylene. **W. Xie**

2:20 CATL **164.** Interfacial chemistry of metal nanocatalysts. **N. Zheng**

2:50 CATL **165.** Influence of co-adsorbates on metal-reducible oxide interfacial sites for selective C-O cleavage reactions. L.V. Herrera, T. Omotoso, N. Briggs, L. Grabow, **S. Crossley**

3:10 Intermission.

3:20 CATL **166.** Engineering the Pt/CeO_2 interface for the development of advanced catalysts. **Y. Xia**

3:50 CATL **167.** *In-situ* transmission electron microscopy with atomic resolution at atmospheric pressure. **X. Pan**, S. Dai, S. Zhang, G. Graham

4:20 CATL **168.** Introducing time resolution to detect Ce^{3+} catalytically active sites at the Pt/CeO_2 interface through ambient pressure x-ray photoelectron spectroscopy. **L. Artiglia**, F. Orlando, K. Roy, R. Kopelent, O. Safonova, M. Nachtegaal, T. Huthwelker, J. van Bokhoven

4:40 CATL **169.** Support-induced control of surface composition in bimetallic catalytic particles. **P. Christopher**

5:10 CATL **170.** Acceptorless dehydrogenation of glycerol by single-site heterogeneous catalysis. **M. Finn**, J. Heltzel, A. Voutchkova

Section E

Walter E. Washington Convention Center
Room 140A

Advanced Electrocatalysis for Energy Conversion & Storage

Electrochemical Conversion of Organic Molecules & other Reactions

A. Holewinski, C. Wang, B. Xu, *Organizers*

A. B. Padmaperuma, *Organizer, Presiding*

C. Wang, *Presiding*

1:30 CATL **171.** Low temperature chemical transformations using electrocatalyst. **J. Holladay**, M. Lilga, A. Padmaperuma, S. Akhade, J. A Lopez-Ruiz, M. Swita, T. Lemmon

2:10 CATL **172.** Exploring catalyst for the ethanol oxidation reaction. **Y. Liu**, C. Wang

2:30 CATL **173.** Deposited Au nanoparticles on high-index facets of PtNi concave-nanocubes for high-performance methanol oxidation reaction. **L. Yu**, Y. Jiang, H. Zhuo, K. Yu, J. Yong, X. Zhang

2:50 Intermission.

3:10 CATL **174.** Computational modeling of electrochemical pyrolysis-oil upgrading. D. Cantu, M. Nguyen, S. Akhade, M. Lee, Y. Wang, Y. Yoon, A. Padmaperuma, M. Lilga, V. Glezakou, **R. Rousseau**

3:50 CATL **175.** Inorganic nanocatalysts for the electronic power circulation using alcohol/carboxylic acid redox couples. **M. Yamauchi**, S. Kitano, M. Sadakiyo

4:10 CATL **176.** Zeolitic imidazolate-frameworks derived nitrogen-doped graphene/cobalt-embedded porous carbon polyhedron hybrid as trifunctional electrocatalyst for oxygen reduction and water splitting. **Y. Hou**, Z. Wen, S. Cui, J. Chen

4:30 CATL **177.** Mechanistic insight into sulfide-enhanced oxygen reduction reaction activity and stability of commercial Pt black: An *in situ* Raman spectroscopic study. **Y. Wang**, D. Chen, Y. Tong

Section F

Walter E. Washington Convention Center
Room 140B

2016 ACS Catalysis Lectureship for the Advancement of Catalytic Science: Honoring Matthias Beller

B. de Bruin, *Organizer, Presiding*

1:30 CATL **178.** New developments in homogeneous hydrogenation. **J.G. De Vries**

1:55 CATL **179.** Earth abundant transition metal catalysis for CO_2 and CO conversion. **T. Skrydstrup**

2:20 CATL **180.** Reductive iron catalysis and nanocluster formation. **A. von Wangelin**

2:45 CATL **181.** C-N and C-C bond formation *via* selective functionalization of saturated cyclic amines. **C. Bruneau**

3:10 Intermission.

3:30 CATL **182.** Site-Selective oxidation, amination and epimerization reactions of complex polyols enabled by transfer hydrogenation. C.K. Hill, **J.F. Hartwig**

3:55 CATL **183.** Metal ligand cooperation in catalyzed dehydrogenations. **H. Grützmacher**

4:20 CATL **184.** Biocatalytic asymmetric amination and C-C bond formation. **W. Kroutil**, N.G. Schmidt, S. Payer, L. Hammerer, S. Velikogne, E. Eger, J. Farnberger, M. Fuchs, J. Pletz, J. Schrittwieser, C. Winkler

4:45 CATL **185.** Building bridges between homogeneous and heterogeneous catalysis: What can we learn from each other? M. Beller

Intellectual Property Considerations When Entering into a Joint Venture

Sponsored by CHAL, Cosponsored by CATL, CELL, ENFL and SCHB

Eminent Scientist Lecture

Sponsored by SOCED, Cosponsored by CATL and POLY

Nano-Enabled Water Treatment Technologies: Applications & Implications

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Energy & Fuels Storch Award in Fuel Science: Symposium in honor of Umit S. Ozkan

Sponsored by ENFL, Cosponsored by CATL

Heterogeneous Catalysis for Environmental & Energy Applications

Sponsored by ENVR, Cosponsored by CATL

MONDAY EVENING

Section A

Walter E. Washington Convention Center
Halls D/E

Sci-Mix

K. K. Ramasamy, *Organizer*

8:00 - 10:00

20, 35, 42, 55, 61, 63, 67, 72, 74, 83-85, 105-106, 112, 118, 131, 163, 170, 177. See previous listings.

235-236, 246, 321, 336, 340, 356, 360, 376, 386, 388, 396, 399, 406, 415, 435, 438, 441-442, 444, 447, 451-452, 461, 463, 472, 478. See subsequent listings.

TUESDAY MORNING

Section A

Walter E. Washington Convention Center
Room 101

Advances in Computational Catalysis

G. Mpourmpakis, R. Surendran Assary, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CATL **186.** Machine learnt molecular simulation models for catalyst design. B. Narayanan, H. Chan, M. Cherukara, **S. Sankaranarayanan**

9:05 CATL **187.** Machine (&Human!) learning in catalyst discovery. Z. Li, S. Wang, **H. Xin**

9:35 CATL **188.** High-throughput workflows for determining adsorption energies on solid surfaces. **J. Montoya**, K. Persson

9:55 CATL **189.** Developing structure activity relationships in the dehydrogenation of alkanes on oxides. **M. Dixit**, G. Mpourmpakis

10:15 Intermission.

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

‡ *Cooperative Cosponsorship*

10:30 CATL **190.** Withdrawn.

11:00 CATL **191.** Heterolytic splitting of molecular hydrogen by frustrated and classical Lewis pairs: A unified reactivity concept. G. Skara, F. De Vleeschouwer, P. Geerlings, F.J. De Proft, **B. Pinter**

11:20 CATL **192.** Mo_2C catalysts for the upgrading of furan in biooil for fuel applications. **D. Pahls**, B. Narayanan, R.S. Assary, L.A. Curtiss

11:40 CATL **193.** Potential energy surface of glucopyranose reactions with hydrogen cation, mechanistic propositions. **M.K. Ghosh**, M.S. Howard, K. Dussan, S. Dooley

12:00 Concluding Remarks.

Section B

Walter E. Washington Convention Center
Room 102B

Emerging Catalytic Processes for Methane Conversion

Cosponsored by ENFL

D. Liu, *Organizer*

E. Hensen, Y. Lei, *Organizers*, *Presiding*

X. Bao, D. Liu, *Presiding*

8:30 CATL **194.** Photocatalytic methane steam reforming over defect-rich TiO_2. **A.M. Pennington**, A. Hook, R.A. Yang, F.E. Celik

8:50 CATL **195.** Characterization of $MoVTeNbO_x$ catalysts during oxidation reactions using *In situ*/*Operando* techniques. **A.M. Gaffney**

9:20 CATL **196.** Partial oxidation of light alkanes by iodine oxides. **T.B. Gunnoe**, J.T. Groves, W.A. Goddard, N. Schwartz, N. Boaz, R. Fu, R.J. Nielsen, G. Fortman, S.E. Kalman

9:50 CATL **197.** New fundamental molecular level insights into oxidative coupling of methane (OCM) by SiO_2-supported tungstate catalysts. M. Zhu, Z. Fink, W. Taifan, M. Ford, F. Tielens, J. Baltrusaitis, **I.E. Wachs**

10:25 Intermission.

10:40 CATL **198.** Fundamental research on direct methane conversion: An industrial perspective. **S. van Bavel**

11:10 CATL **199.** Modular chemical process intensification: Enabler for gas conversion. **J. Bielenberg**

11:40 CATL **200.** Direct methane conversion to aromatics. Y. Liu, T. Wang, **T. Xu**, Y. Zhang

12:10 CATL **201.** Methane dehydroaromatization over Mo/ZSM-5 catalyst: Effect of residual charge on reaction energy profiles of Mo_4C_2 and Mo_2C_6 nanoclusters. T. Khan, S. Mishra, S. Balyan, K.K. Pant, **M. Haider**

Section C

Walter E. Washington Convention Center
Room 102A

Metal-Support Interactions in Catalysis: Modeling, Characterization & Design

A. Baber, A. Bruix, S. D. Senanayake, *Organizers*

T. Duchon, *Presiding*

8:30 CATL **202.** Nanoparticle synthesis via electrostatic adsorption using incipient wetness impregnation. **S. Eskandari**, J.R. Regalbuto

8:50 CATL **203.** Unbiased photocatalytic hydrogen generation from pure water on stable Ir-treated $In_{0.33}Ga_{0.67}N$ nanorods. M. Ebaid, T. Isimjan, T. Ng, B. Ooi, **H. Idriss**

9:25 CATL **204.** Mechanistic studies of oxidation reactions on supported vanadia catalysts. **E. Weitz**, W. Wu, K. Ding, T. Drake, S. Kwon, P.C. Stair

10:00 Intermission.

10:15 CATL **205.** Modifying surface coverage to improve WGS activity and sulfur-dependence of ZrO_2 supported Mo catalysts. **S. Yun**, V.V. Guliants

10:35 CATL **206.** Topotactic growth of edge-terminated MoS_2 from MoO_2 nanocrystal surfaces. **M. Brorson**, C. Dahl-Petersen, M. Šarić, P. Moses, J. Rossmeisl, J. Lauritsen, S. Helveg

11:10 CATL **207.** Catalytic aromatization of methane: Strategies for improving active chemistry, mitigation of coke formation and sustaining selectivity to benzene. **S. J. Khatib**, M. Rahman, A. Sridhar, J. Tata, L. Harper

11:45 CATL **208.** Enhanced higher alcohol synthesis via tuning the metal-support interaction using surfactant-encapsulated polymolybdate precursor. J. Yong, X. Luan, **X. Dai**, H. Qiao, Y. Yang, Y. Zhang, X. Zhang

Section D

Walter E. Washington Convention Center
Room 103B

Cooperative Catalysis at Surfaces & Interfaces: Impact on Chemistry & Energy Frontiers

Metal Catalysis

Cosponsored by ENFL

M. Cargnello, Z. Wu, *Organizers*

S. Zhang, *Organizer, Presiding*

M. Cargnello, *Presiding*

8:30 CATL **209.** Catalytic action at a distance: Hydrogen spillover over oxidic surfaces. **J.A. Van Bokhoven**

9:00 CATL **210.** Identifying the active surface in bimetallic RuSn hydrogenation catalysts and the role of Sn. **V. Vorotnikov**, T.R. Eaton, A. Settle, E. Wegener, C. Yang, J.T. Miller, G. Beckham, D. Vardon

9:20 CATL **211.** PdZn catalysts for the direct hydrogenation of CO_2 to methanol. H. Bahruji, M. Bowker, G. Hutchings, W. Jones, D. Morgan, **R.D. Armstrong**

9:50 CATL **212.** In situ synthesis of porous graphitic carbon nanosheets with immobilized ultra-fine PtNi intermetallic nanoparticles: Their outstanding catalytic capability for *p*-nitrophenol hydrogenation. **J. Zhang**

10:10 Intermission.

10:25 CATL **213.** Promoting aldol addition by cooperative interactions in metal functionalized chitosan. C. Khoury, D. Shpasser, **O. Gazit**

10:55 CATL **214.** Rational design of nanostructured supported catalysts for environmental and energy applications. **T. Shirman**

11:15 CATL **215.** Effects of TiO_2 in low temperature propylene epoxidation using Au/SiO_2 catalysts. Z. Lu, Z. Wu, C. Turner, **Y. Lei**

11:45 CATL **216.** Tailoring of metal-oxide interface by atomic layer deposition. **B. Zhang**, H. Liang, Y. Qin

12:05 Concluding Remarks.

Section E

Walter E. Washington Convention Center
Room 140A

New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics

B. Ginovska, M. J. O'Hagan, *Organizers*

S. Raugei, *Organizer, Presiding*

8:30 CATL **217.** Radical mechanism of the nickel enzyme methyl-CoM reductase, which catalyzes the synthesis and activation of methane. **S.W. Ragsdale**, A. Patwardhan, T. Wongnate, B. Ginovska, M. Wolf, L.J. Giles, J. Mock, P. Pimviriyakul, N. Lehnert, S. Raugei, R. Sarangi

8:55 CATL **218.** Insights on the mechanism of H_2 activation by [FeFe]-hydrogenases. **P.W. King**, D.W. Mulder, Y. Guo, M. Ratzloff

9:20 CATL **219.** Electrocatalytic diversity of hydrogenases. **A.K. Jones**, S. Williams, Z. Nazemi, P. Kwan, J. Artz, C. McIntosh, D.W. Mulder, M. Ratzloff, P.W. King, M.W. Adams, J. Peters

9:45 CATL **220.** Probing transient states in the catalytic cycle of [FeFe]-hydrogenases. **M. Winkler**, J. Duan, J. Esselborn, L. Kertess, D. Adam, U. Apfel, S.T. Stripp, T. Happe

10:10 Intermission.

10:25 CATL **221.** Statistical fluctuations, dynamics, scaffolds, electric fields, and de novo enzyme catalysis. **T.L. Head-Gordon**

10:50 CATL **222.** Small molecule activation: Nitrogenase as paradigm. **B.M. Hoffman**

11:15 CATL **223.** Modulation of electron transfer in nitrogenase. **L.E. Johnson**, B. Ginovska, S. Raugei

11:35 CATL **224.** Mechanistic insights into energy conservation by flavin-based electron bifurcation. **J. Peters**, C. Lubner, D.P. Jennings, D.W. Mulder, G.J. Schut, O. Zadvornyy, J.P. Hoben, M. Tokmina-Lukaszewska, L. Berry, D. Nguyen, G. Lipscomb, B. Bothner, A.K. Jones, A.F. Miller, P.W. King, M.W. Adams

Section F

Walter E. Washington Convention Center
Room 140B

Multimodal Characterization of Functional Energy Materials

Analyses

Cosponsored by ENFL

N. Rajput, *Organizer*

V. Murugesan, L. Trahey, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CATL **225.** Accelerating materials design and optimization for battery materials with a multi-modal approach. **K.T. Mueller**, K. Han, V. Murugesan, J.Z. Hu, N. Rajput, K. Persson

9:05 CATL **226.** Structural characterizations with combined x-ray techniques in energy storage material applications. **X. Xiao**, Q. Liu, Y. Sun, C. Sun, Y. Ren, W. Liu, R. Xu, L. Trahey

9:35 CATL **227.** Towards understanding and enabling magnesium batteries. **R. Mohtadi**, O. Tutusaus, T.S. Arthur

10:05 CATL **228.** Expanding the scope of *in situ* techniques to probe amorphous electrocatalysts. **N. Kornienko**, P. Yang, E. Reisner

10:20 Intermission.

10:35 CATL **229.** In-situ/operando multimodal soft x-ray characterization in energy science. **J. Guo**

11:05 CATL **230.** *In situ and ex situ* NMR for battery research. **J.Z. Hu**, M. Hu, C. Wan, V. Murugesan, J. Zhang, K.T. Mueller

11:35 CATL **231.** Multi-modal *operando* investigations of activities and phase transformations of supported Pd nanocatalysts during ethylene hydrogenation reaction. **Y. Li**, S. Zhao, D. Liu, A. Orlov, R.G. Nuzzo, E. Stach, A. Frenkel

11:50 CATL **232.** Chemical imaging of redox active molecules in SEI layer of Li-S batteries using in-situ x-ray photoelectron spectroscopy. **M. Nandasiri**, A.M. Schwarz, V. Shutthanandan, L.E. Camacho-Forero, P.B. Balbuena, T. Thevuthasan, K.T. Mueller, V. Murugesan

12:05 CATL **233.** Magnetically interactive hierarchical assembly of $GaFeO_x$ decorated vertically aligned ZnO nanorod arrays for enhanced visible photocatalytic activity. R. Kugalur Shanmugam, N. L Raveendran, **R. Rajendrakumar**

Nano-Enabled Water Treatment Technologies: Applications & Implications

Sponsored by ENVR, Cosponsored by CATL

TUESDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 101

Advances in Computational Catalysis

G. Mpourmpakis, *Organizer*

R. Surendran Assary, *Organizer, Presiding*

1:00 Introductory Remarks.

1:05 CATL **234.** Density functional theory study of oxygen reduction reaction on non-precious transition metal/nitrogen doped carbon catalysts. K. Liu, **G. Wang**

1:35 CATL **235.** Dehydrogenation mechanisms on γ-alumina supported platinum subnanometric-clusters: A DFT approach coupled with experimental kinetics study. **W. Zhao**, C. Chizallet, P. Galguen, J. Verstraete, J. Lavy, P. Sautet, P. Raybaud

TECHNICAL PROGRAM

1:55 CATL **236.** Elucidating and correcting the unreliability of continuum solvation methods when modeling homogeneous reaction mechanisms. **Y. Basdogan**, J.A. Keith

2:15 CATL **237.** Developing iridium-based alloys as effective catalysts by the combination of density functional theory and cluster expansion method. **L. Mehdizadegan Namin**, N.A. Deskins, K. Yuge

2:35 Intermission.

2:50 CATL **238.** Theoretical insights into the effects of oxidation and transition metal-doping on the structure and properties of Pt-Ni nanocatalysts. **L. Cao**, T. Mueller

3:10 CATL **239.** Engineering ligand-protected Au nanoclusters for CO_2 reduction. **N. Austin**, G. Mpourmpakis

3:30 CATL **240.** Reaction mechanism of the selective reduction of CO_2 to CO by a tetraaza $[Co^{II}N_4H(MeCN)]^{2+}$ complex. **A.J. Garza**, O.O. Iyiola, J.L. Mendoza-Cortez, A.T. Bell, M.P. Head-Gordon

3:50 CATL **241.** DFT study of biomimetic CO_2 hydration over M-$C_{95}H_{26}$/M-N_3-$C_{92}H_{26}$ graphene. **M. Verma**, P. A. Deshpande

4:10 Concluding Remarks.

Section B

Walter E. Washington Convention Center
Room 102B

Vehicle Emission Control Catalysis: New Era, New Challenges & New Solutions

Cosponsored by ENFL and ENVR

F. Gao, C. H. Peden, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 CATL **242.** Challenges and solutions in diesel NOx emission control. **H. Chen**

1:45 CATL **243.** Consequences of Cu ion mobility in zeolites for low temperature NOx SCR with ammonia. C. Paolucci, A. Parekh, I. Khurana, J. Di Iorio, A. Shih, H. Li, S. Li, A. Yezerets, W. Delgass, J.T. Miller, F. Ribeiro, W.F. Schneider, **R. Gounder**

2:25 CATL **244.** Sulfur poisoning and removal of Cu/SSZ-13 SCR catalyst. **J. Luo**

2:45 Intermission.

3:05 CATL **245.** Towards atomic level understanding of the transformation of Cu active sites in Cu/SSZ-13 selective catalytic reduction catalysts during hydrothermal aging. **Y. Wang**, J. Song, E.D. Walter, N.M. Washton, D. Mei, L. Kovarik, Y. Wang, F. Gao, C.H. Peden

3:25 CATL **246.** Mechanistic study of S poising in Cu-SSZ-13: Responses of Cu^{2+} and CuOH active centers to SO_2 exposure. **Y. Jangjou**, D. Wang, A. Kumar, J. Li, W.S. Epling

3:45 CATL **247.** New insights into NH_3/NO chemisorption properties and NH_3-SCR reaction mechanism over Cu/SAPO-34 as NH_3-SCR catalysts. **L. Wang**, W. Li, G. Qi, D. Weng

4:05 CATL **248.** Pt/B-graphene catalyst for low temperature H_2-SCR. **Z. Yao**, M. Hu, X. Wang

Section C

Walter E. Washington Convention Center
Room 102A

Advances in Carbon Dioxide Utilization

Cosponsored by ENFL and ENVR

V. Abdelsayed, *Organizer*

F. Jiao, F. Shi, *Organizers*, *Presiding*

1:00 CATL **249.** Molecular heterogeneous electrocatalyst materials for carbon dioxide reduction. **H. Wang**

1:30 CATL **250.** High performance CO_2 electrolyzers. **J.P. Baetzold**, C. Hartmann-Thompson, M. Kaplun, N. Kunz, K. Lewinski, D. Lutz, L. Nereng, M.J. Pellerite, Z. Liu, H. Yang, R. Masel

1:50 CATL **251.** Li electrochemical tuning of metal oxide for highly selective aqueous CO_2 reduction. **K. Jiang**, H. Wang

2:10 CATL **252.** Solid oxide co-electrolysis of steam and CO_2 to unlock a renewable energy based synthetic fuel economy. **J.J. Hartvigsen**, S. Elangovan, J. Elwell, L. Frost

2:30 Intermission.

2:45 CATL **253.** Snapshots of the CO_2 electroreduction pathways using effects of electrolyte and pyridine. **I. Chernyshova**, P. Somasundaran, M. Goldman, S. Yi Wang, S. Ponnurangam

3:05 CATL **254.** Ligand-functionalized gold as versatile and tunable electrocatalysts for CO_2 reduction. Y. Fang, X. Cheng, **Y. Xu**, J.C. Flake

3:25 CATL **255.** Withdrawn.

3:45 CATL **256.** Cyborg bacteria: Inorganic-biological hybrid organisms for solar-to-chemical production. **K.K. Sakimoto**, P. Yang

4:05 CATL **257.** High-selectivity, biocatalytic gas fermentation of CO_2 to ethanol. **R. Conrado**

Section D

Walter E. Washington Convention Center
Room 103B

Nanoporous Materials for Catalysis in Global Economy

E. Kyriakidou, Z. Li, D. Liu, H. Wang, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 CATL **258.** Ion mobility and site pairing in zeolite catalysis. **W.F. Schneider**

1:40 CATL **259.** Copper mobility in zeolite-based SCR catalysts. **M. Skoglundh**, S. Shwan, L. Chen, P.N. Vennestrøm, T.V. Janssens, L.F. Lundegaard, R.R. Tiruvalam, A. Carlsson, J. Jansson, H. Gronbeck

2:05 CATL **260.** Environmental sensitivity of spectroscopic properties for Cu ions in Cu-SSZ-13: XANES and XES studies from first principles. R. Zhang, H. Li, K. Groden, J. Szanyi, F. Gao, S.L. Scott, **J. McEwen**

2:30 CATL **261.** Chemical poisoning of Cu/SSZ-13 used for ammonia selective catalytic reduction. K. Xie, K. Wijayanti, A. Kumar, K. Kamasamudram, **L. Olsson**

2:55 Intermission.

3:15 CATL **262.** Low-Temperature Pd/zeolite passive NOx adsorbers: Structure, performance and adsorption chemistry. **F. Gao**, Y. Zheng, L. Kovarik, M. Engelhard, J. Szanyi

3:45 CATL **263.** One-step dual template synthesis and catalytic characterization of hierarchical lamellar zeolite composite materials. **D. Liu**, L. Emdadi

4:10 CATL **264.** Hydrophilicity/hydrophobicity modulating zeolite synthesis: nanocrystals or hierarchically structured materials. **Z. Hua**

4:35 Concluding Remarks.

Section E

Walter E. Washington Convention Center
Room 140A

New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics

B. Ginovska, S. Raugei, *Organizers*

M. J. O'Hagan, *Organizer, Presiding*

1:00 CATL **265.** Artifical metalloproteins: Developing methods to control the local environments around metal ions. **A. Borovik**, S.I. Mann, L. Olshansky

1:25 CATL **266.** Unmasking the interplay of redox-active and hemilabile ligands in proton reduction electrocatalysis: Computationally derived mechanisms. **M.B. Hall**

1:50 CATL **267.** Unmasking the interplay of redox-active and hemi-labile ligands in proton reduction electrocatalysis: Synthesis and characterization of a matrix of MN_2S_2-M' complexes. P. Ghosh, M. Quiroz, S. Ding, M.B. Hall, **M.Y. Darensbourg**

2:15 CATL **268.** Artifical enzymes: Attaching a protein-like scaffold on molecular catalysis is essential for high efficiency. A. Dutta, N. Boralugodage, **W.J. Shaw**

2:40 Intermission.

2:55 CATL **269.** Chemical and electrochemical probes for H2 and H+ in amine-complemented HER catalysts. **T.B. Rauchfuss**, N. Lalaoui

3:20 CATL **270.** Structural + functional models of mono-iron hydrogenase featuring an anthracene scaffold ligand. **M.J. Rose**, J. Seo, T. Manes, S. Kerns, E. Sullivan

3:45 CATL **271.** New ligand frameworks for catalysis inspired by the active site of enzymes. **J.Y. Yang**, J. Khosrowabadi Kotyk, T. Chantarojsiri, A. Reath, J. Barlow, R. Combs

4:10 CATL **272.** Accelerating the first-principles discovery of biomimetic catalysts. **T.Z. Gani**, J. Janet, H.J. Kulik

Section F

Walter E. Washington Convention Center
Room 140B

Multimodal Characterization of Functional Energy Materials

Measurement & Modeling

Cosponsored by ENFL

N. Rajput, L. Trahey, *Organizers*

V. Murugesan, *Organizer, Presiding*

R. Rajendrakumar, *Presiding*

1:30 CATL **273.** Signatures of inhomogeneous sulfur loading in microporous carbon-based electrodes from molecular dynamics and x-ray absorption spectroscopy. **D. Prendergast**, T.A. Pascal, I. Villaluenga, K. Wujcik, X. Jiang, D. Devaux, R. Wang, N.P. Balsara

2:00 CATL **274.** Characterization of solvation and reaction effects at the Li-metal/electrolyte interface. **P.B. Balbuena**, L.E. Camacho-Forero, E. Kamphaus, F.A. Soto, V. Murugesan

2:30 CATL **275.** Integrating first principles modeling with multimodal interrogation of hybrid Li-ion/Li-O_2 battery materials. **M. Chan**

3:00 CATL **276.** Simultaneous in-situ neutron diffraction and thermogravimetric analaysis of iron catalysts under ammonia decomposition conditions. **T. Wood**, W. David, J. Makepeace

3:15 Intermission.

3:30 CATL **277.** Exploring electron delocalization on the femtosecond timescale. **N. Govind**, A. Andersen, Z. Fox, Y. Zhang, S. Mukamel, M.H. Khalil

4:00 CATL **278.** Multiscale computational studies of solid species formation in chemical transformation batteries. **L. Cheng**, L.A. Curtiss, P. Redfern, R.S. Assary, K. Lau

4:30 CATL **279.** Multimodal characterization of solid acid catalyst active sites for hydrocarbon upgrading. A. Wang, L. Sharma, G.X. Yan, M. Ford, I.E. Wachs, **J. Baltrusaitis**

4:45 CATL **280.** Predicting mesoscale chain properties of electronically excited conjugated polymers. **B. Wood**, Y. Shin, K. Persson

5:00 CATL **281.** Adsorption characteristics of lithium polysulfides Li_2S_x (x=2 to 8) on 2D surfaces. **S. Lakshmipathi**, A. Arokiyanathan, A. Balasubramanian

Nano-Enabled Water Treatment Technologies: Applications & Implications

Sponsored by ENVR, Cosponsored by CATL

TUESDAY EVENING

Section A

Walter E. Washington Convention Center
Hall D

General Catalysis

S. Subramaniam, *Organizer*

6:00 - 8:00

CATL **282.** Size-dependent activity of CrO_3 in catalyzing NO oxidation: From the inert bulk structure to highly efficient supported chain-like CrO_3. **J. Jin**, H. Wang, P. Hu

CATL **283.** Octanoic acid catalytic hydrogenation over Ni nanoparticles embed in 3D ordered macroporous ZrO2: The effect of catalysts structure. **H. Chen**

CATL **284.** Formation of novel g-C_3N_4@ $ZnIn_2S_4$ composite heterojunction nanosheet with a outstanding photocatalytic hydrogen evolution activity. **B. Lin**

CATL **285.** Studying the roles of transition metals on converting methane to value-added methanol. **C. Zhang**

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

‡ *Cooperative Cosponsorship*

CATL **286.** Heterogeneous dephosphorylation of biomolecules via ceria nanocatalysts. M. Manto, P. Xie, **W. Liano**, C. Wang

CATL **287.** CO_2 Reduction through dry reforming reaction with methane over supported Fe-Ni bimetallic and Fe-Ni-Mo trimetallic heterogeneous catalysts. **A. Tripoli**, C. Zhang

CATL **288.** Liquid-phase partial oxidation of methane into oxygenates with H_2O_2. M. Kim, **E. Park**

CATL **289.** Withdrawn.

CATL **290.** Withdrawn.

CATL **291.** Novel nanoporous N-doped carbon-supported ultrasmall Pd nanoparticles: Efficient catalysts for hydrogen storage and release. **K. Koh**, M. Jeon, D. Chevrier, C. Yoon, P. Zhang, T.G. Asefa

CATL **292.** Influence of different elemental ratios and thermal pretreatment on the aromatization of propane using Ga-Al-MFI catalyst. **M.N. Akhtar**, S. Asaoka

CATL **293.** Cost-effective fabrication and improved photodegradation activities of bismuth vanadate/bismuth oxychloride composite. **J. Pu**, N. Zhang, Y. Chen

CATL **294.** Design of interface for transfer hydrogenation catalysts. **Y. Zhou**, Y. Kang

CATL **295.** Controlled construction of single-atom catalysts via molecular monolayers modification. **X. Fu**, Y. Kang

CATL **296.** Enhancing electrocatalytic properties of molybdenum disulfide for hydrogen evolution reaction via anion doping. **G. Qu**, Y. Kang

CATL **297.** Effect of catalytic structure on hydrogenolysis of microalgae (*spirulina sp.*) polysaccharide into polyols over zeolites-supported Platinum catalysts. **M. Gu**, Z. Shen, W. Dong, Y. Zhang

CATL **298.** Design of multimetallic alloy catalysts for CO_2 reduction. **R. Zhang**, Y. Kang

CATL **299.** Modification of valence band of ceria via anion doping with fluorine. **M. Kettner**, T. Duchon, M. Wolf, J. Kullgren, P. Kus, K. Sevcikova, Z. Rafaj, K. Hermansson, V. Nehasil

CATL **300.** Room temperature removal of NO on MnO_2: First principles calculations combined with kinetic analysis. **H. Yuan**, J. Chen, H. Wang, P. Hu

CATL **301.** In-situ growth of high-density $Zn_{0.2}Cd_{0.8}S$/NiS nanoparticles on graphene nanosheets as tandem nanoreactor for efficient hydrogen evolution. **C. Xue**

CATL **302.** Structure composition and shape tunable PtAuNi nanoparticles for electroctalytic oxidation of methanol. **A. Lu**, D. Peng, D. Zeng, Z. Skeete, H. Zheng, S. Yan, A. Sharma, F. Chang, J. Luo, V. Petkov, C. Zhong

CATL **303.** Developing new catalytic application of doping-segregation method for selective CO_2 conversion. **Q. Wu**, B. Yan, J. Cen, E. Stach, A. Frenkel, J.G. Chen, A. Orlov

CATL **304.** Difunctional magnetic Pd/TiO_2@SiO_2@Fe_3O_4 catalysts and methanol catalytic conversion to formic acid and methyl formate. **S. Ji**

CATL **305.** Influence of *OH adsorbates on the potentiodynamics of the CO_2 generation during the electro-oxidation of ethanol. **G. Yang**, N.A. Deskins, X. Teng

CATL **306.** Epimerization of isosorbide to isoidide using Ru/NiO–TiO_2 catalyst. **J. Hwang**, J. Jegal

CATL **307.** CO_2 reduction through dry reforming reaction with methane over supported Cu-Ni bimetallic and Cu-Ni-Pd trimetallic heterogeneous catalysts. **L. Jiao**, C. Zhang

CATL **308.** Dry reforming of CO_2 with methane over supported CoNi bimetallic and CoNiPd trimetallic catalysts. **S. Bamonte**, C. Zhang

CATL **309.** CO_2 reduction through dry reforming reaction with methane over supported Ni-Pd bimetallic and Ni-Mo-Pd trimetallic heterogeneous catalysts. **S. Mirabelli**, C. Zhang

CATL **310.** Oxidative dehydrogenation of ethane to ethylene over molybdenum-vanadium based catalysts. **S. Samangain**, B. Kitiyanan, S. Pengpanich, K. Thavornprasert

CATL **311.** Multimodal approaches to understanding protective barriers in lithium-sulfur batteries. **B.C. Wilson**, R.A. Nye, R. Iuliucci, V. Murugesan, K.T. Mueller

CATL **312.** CO_2 conversion via nanoporous PS-PVP block copolymer: Revisiting the pyridyl radical. **H. Ghebremichael**, A. Sidorenko

CATL **313.** Ag nanoparticles and graphitic carbon nitrides co-decorated TiO_2 nanocomposites for enhanced photocatalytic activity under visible light. **H. Tian**

CATL **314.** Hydrolysis of a chemical warfare agent simulant by a Zr-containing polyoxometalate: Rate enhancement in the presence of acetate buffer. **D.L. Collins-Wildman**, M. Kim, K.P. Sullivan, C.L. Hill

CATL **315.** Metal-organic frameworks as models of metal oxides supports for catalytic hydrogenation of CO_2. **B. An**, J. Zhang, K. Cheng, C. Wang, W. Lin

CATL **316.** Concave Bi_2WO_6 nanoplates with oxygen vacancies achieving enhanced electrocatalytic and photocatalytic activitie. **M. Dekun**

CATL **317.** Polyoxometalate stabilized ruthenium nanoparticles supported on nanohydrotalcite: Highly efficient nanocatalyst for the oxidation of lignin model compounds. **M. Zahmakiran**, B. Baguc, M. Celebi

CATL **318.** Photophysical characterization of photocatalytic Rhenium(I) materials for CO_2 reduction. **J. Martin**, R.W. Larsen

CATL **319.** Study of Cu-based catalysts for methane to methanol electro-oxidation reaction. **H. Ataee-Esfahani**, D. Chen, Y. Tong

CATL **320.** Homogeneous catalysis of hydrolysis of phosphate esters by Schiff base transition metal complexes. **U. Okeke**, R.N. Egekenze, R. Butcher, Y. Gultneh

CATL **321.** Commercially available novel H-bonding catalyst for ring opening polymerization of lactones. **N. Dharmaratne**, J. Pothupitiya, T.J. Bannin, O.I. Kazakov, M.K. Kiesewetter

CATL **322.** Probing nanoscale heterogeneous electrode interface using tip-enhanced Raman spectroscopy. **G. Kang**, M. Mattei, G. Goubert, G.C. Schatz, R.P. Van Duyne

CATL **323.** Liquid-gas interface explored by ambient pressure x-ray photoelectron spectroscopy. **L. Artiglia**, F. Orlando, S. Chen, K. Roy, I. Gladich, J.A. Van Bokhoven, M. Ammann

CATL **324.** Mn(II) complexes, $[Mn_2(\mu\text{-}R_1C_6H_3COO)_2(R_2)_4].2(ClO_4)$, ($R_1$:Cl, NH_2, CH_3); R_2:1,10'-phenanthroline or 2,2'-bipyridine): Synthesis, oxidation of alcohols/alkenes and catalase activity. **I. Avan**, Y. Kilic, I. Kani

CATL **325.** Homogeneous oxidation of alcohols in water catalyzed by a Cu(II) complex with a triphenyl acetate/bipyridyl ligands. H. Ünver, **I. Kani**

CATL **326.** Transition metal-based alloy and core-shell nanowire electrocatalysts for the oxidation of small organic molecules. **R. Marquez Valencia**, I. Colliard, G. Singh, T.J. Aimola, A. Kassotis, N. Smina, C. Koenigsmann

CATL **327.** Enhanced electrocatalytic oxygen reduction and methanol oxidation performance in hollow Pt-Ag nanoparticles. **G. Singh**, T.J. Aimola, S. Chen, S. Thota, J. Zhao, C. Koenigsmann

CATL **328.** First principle study of optical, electronic, magnetic and catalytic properties of p-elements doped TiO_2 surface. **A. Aldakheel**

CATL **329.** DFT simulation of nitrogen-doped graphene as an ORR catalyst in fuel cells. **G. Arias**, N. Humphrey, W.A. Goddard, T. Yu

CATL **330.** Withdrawn.

CATL **331.** Chiral transition metal diphosphine complexes and their applications in asymmetric catalysis. **S. Lorraine**, P.T. Maragh, T. Dasgupta, K. Abdur-Rashid

CATL **332.** Important of biotechnological processes. **T.D. Komolafe**

CATL **333.** Development of machine-learning chemisorption models for oxide electrocatalysis. **Z. Li**, H. Xin

CATL **334.** Withdrawn.

CATL **335.** Catalyst in poultry nutrition. **T.O. Akinmusire**

CATL **336.** General approach to M/Au (M = Fe, Cu) core/shell and Ni/Au core/satellite nanoparticle. **X. Liu**, G. Lu, S. Dai, H. Zhu

WEDNESDAY MORNING

Section A

Walter E. Washington Convention Center
Room 101

Advances in Computational Catalysis

R. Surendran Assary, *Organizer*

G. Mpourmpakis, *Organizer, Presiding*

8:30 Introductory Remarks.

8:35 CATL **337.** Improving solvation models for electrochemistry. **K. Schwarz**, R. Sundararaman

8:55 CATL **338.** DFT simulation of edge halogenated nanosheets as an ORR catalyst in fuel cells. **N. Humphrey**, R. Rodriguez, G. Arias, T. Yu, W.A. Goddard

9:15 CATL **339.** Theoretical insights into the role of water in heterogeneous catalysis. **C. Chang**, J. Li

9:35 Intermission.

9:50 CATL **340.** Assessing the thermodynamic landscape for cobalt catalyzed CO_2 reduction. **I.M. Pendleton**, P.M. Zimmerman

10:10 CATL **341.** Comparing the oxygen reduction reaction on armchair and zigzag edges from quantum mechanics. **T. Yu**, L. Quang, W.A. Goddard

10:30 CATL **342.** First-principles kinetic Monte Carlo simulation of CO oxidation on PdO(101). **M. Kim**, A.R. Asthagiri

10:50 CATL **343.** Deoptimizing oxygen reduction reaction catalysis with doped amorphous Ti oxides. **M.C. Groenenboom**, J.A. Keith

11:10 CATL **344.** Developing computational methods to reveal fundamental reaction sequences on surfaces. **M. Jafari**, P.M. Zimmerman

11:30 Concluding Remarks.

Section B

Walter E. Washington Convention Center
Room 102B

Vehicle Emission Control Catalysis: New Era, New Challenges & New Solutions

Cosponsored by ENFL and ENVR

F. Gao, C. H. Peden, *Organizers*, *Presiding*

8:30 CATL **345.** Multi-functional structured catalysts for NOx reduction from lean burn vehicles. **M.P. Harold**

9:10 CATL **346.** Withdrawn.

9:30 CATL **347.** Ambient temperature NO oxidation over Cr-based amorphous mixed oxide catalysts: Effects from the second oxide components. A. Wang, Y. Guo, C.H. Peden, **F. Gao**

9:50 Intermission.

10:10 CATL **348.** Response characteristics of pre-commercial mixed potential NO_x and NH_3 sensors in diesel engine exhaust. **C. Kreller**, V.Y. Prikhodko, J. Pihl, S. Curran, K. Ramaiyan, R. Mukundan, J. Parks, E.L. Brosha

10:30 CATL **349.** *In situ* x-ray absorption spectroscopy of bimetallic gold–nickel nanoparticle catalyst for the CO + NO reaction. **S.K. Beaumont**

10:50 CATL **350.** Direct NOx decomposition over oxide catalysts: Advances and perspectives. **C.A. Roberts**, T.C. Peck, G.K. Reddy, H. Jia

11:10 CATL **351.** Application of adsorption-compression theory in gas phase heterogeneous catalytic reaction: Promising proof through direct NO decomposition over Cu-ZSM-5. **P. Xie**, T. Pu, C. Wang

Section C

Walter E. Washington Convention Center
Room 102A

Advances in Carbon Dioxide Utilization

Cosponsored by ENFL and ENVR

F. Jiao, *Organizer*

V. Abdelsayed, F. Shi, *Organizers*, *Presiding*

8:30 CATL **352.** Novel nanoscale hybrid materials for combined CO_2 capture and conversion. M. Gao, **A.A. Park**

9:00 CATL **353.** Development of catalytic process for CO_2 utilization. **H. Lin**

9:20 CATL **354.** Efficient, small catalytic reactor for CO_2 conversion to value-added chemicals. **K. Hawley**, C. Junaedi, S. Roychoudhury

9:40 CATL **355.** Withdrawn.

10:00 CATL **356.** Silica based magnetically retrievable nanocatalysts for CO_2 fixation at ambient conditions. **R. Gaur**

10:20 Intermission.

10:35 CATL **357.** Carbon dioxide as hydrogen vector – the key compounds in storage and delivery: Formic acid and methanol. **G. Laurenczy**

10:55 CATL **358.** Bimetallic Pd-Cu catalysts for CO_2 hydrogenation to methanol. **X. Jiang**, N. Koizumi, X. Guo, C. Song

11:15 CATL **359.** Withdrawn.

11:35 CATL **360.** Carboxylation of propylene oxide to propylene carbonate. **P. Bobba**, B. Subramaniam, R. Chaudhari

11:55 CATL **361.** Influence of Ti/Li/Al-hydrotalcite-like with orientations of crystal growth on its adsorption properties of carbon dioxide. **Y. Dong**, **A. Zhou**, D. Lei, T. Kong

Section D

Walter E. Washington Convention Center
Room 103B

Nanoporous Materials for Catalysis in Global Economy

E. Kyriakidou, Z. Li, D. Liu, H. Wang, *Organizers*, *Presiding*

8:30 Introductory Remarks.

8:35 CATL **362.** Withdrawn.

9:00 CATL **363.** Fabrication of Lewis acid Sn-BEA with tunable hydrophobicity and morphology for cellulosic sugar isomerizations. **W. Fan**, H. Cho

9:25 CATL **364.** Key considerations for designing zeolite catalysts for biomass conversion reactions. **T.C. Hoff**, D.W. Gardner, R. Thilakaratne, R.C. Brown, J. Tessonnier

9:50 CATL **365.** Olefin formation mechanisms of methanol-to-hydrocarbon reactions in H-MFI zeolites. P. Kravchenko, M. DeLuca, **D. Hibbitts**

10:15 Intermission.

10:35 CATL **366.** Resolving zeolite catalysis at the single particle and single turnover level. **M. Roeffaers**

11:00 CATL **367.** Catalytic comparison of nanoporous gold and supported bimetallic gold nanoparticles on a templated nanoporous structure. **J. Lattimer**, T. Shirman, M. Luneau, R.J. Madix, J. Aizenberg, C.M. Friend

11:25 CATL **368.** Naphthalene hydrogenation over noble metal supported on new mesoporous zeolites with high sulfur tolerance. N. Baxter, G. Kuo, **S. Wang**

11:50 CATL **369.** Ambient oxidation of ultrasmall platinum nanoparticles. R. Banerjee, Q. Liu, J. Tengco, **J.R. Regalbuto**

12:15 Concluding Remarks.

Section E

Walter E. Washington Convention Center
Room 140A

New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics

M. J. O'Hagan, S. Raugei, *Organizers*

B. Ginovska, *Organizer, Presiding*

8:30 CATL **370.** Mutational mimics of allosteric effectors to customize enzyme-substrate affinity. **A. Fenton**

8:55 CATL **371.** Metalloenzyme design. **A. Alexandrova**

9:20 CATL **372.** Coupled dynamics in protein allosteric mechanisms from an atomistic perspective. **D. Hamelberg**

9:45 CATL **373.** Molecular mechanism of splicing: An evolutionary computational journey from ribozymes to the spliceosome. **A. Magistrato**

10:10 Intermission.

10:25 CATL **374.** Catalysis by natural and engineered glycosidases. An atomistic view from QM/MM simulations. **C. Rovira Virgili**

10:50 CATL **375.** Inspiration from biology: Coupling electrons and protons and facilitating tunneling. **S. Hammes-Schiffer**

11:15 CATL **376.** Novel scanning electrochemical microscope based method for studying enzymatic proton-coupled electron transfer. **R. Penhallurick**, D. Chen, Y. Tong

11:35 CATL **377.** Connecting catalysis to light-driven electron transfer in photosynthetic hybrids. **D.M. Tiede**, L.M. Utschig-Johnson, K.L. Mulfort

Section F

Walter E. Washington Convention Center
Room 140B

Multimodal Characterization of Functional Energy Materials

Exploration of Interfacial Processes

Cosponsored by ENFL

V. Murugesan, N. Rajput, L. Trahey, *Organizers*

A. Devaraj, S. Lakshmipathi, *Presiding*

8:30 CATL **378.** Combining tender ambient pressure XPS with theory to unravel the solid/liquid electrochemical interface. **E. Crumlin**

9:00 CATL **379.** Multimodal x-ray characterization of solar fuels catalysts under operation. M. Farmand, J. Feaster, R. Davis, S. Fackler, A. Landers, J. Lin, C. Hahn, T.F. Jaramillo, J. Yano, A. Mehta, **W. Drisdell**

9:30 CATL **380.** Simulation and characterization of aluminum-oxide speciation at the water-Mica interface. **M.D. Baer**, C.J. Mundy, A. Tuladhar, J. DeYoreo, B. Legg

10:00 CATL **381.** Challenges in pulsed field gradient NMR on heterogeneous interfaces: Sequence and field dependent diffusion coefficients. **K. Han**, E.W. Hagaman, K.T. Mueller

10:15 Intermission.

10:30 CATL **382.** Optical, morphological, and electrochemical multimodal characterization for integrated $BiVO_4$ photoanodes. G. Liu, J. Eichhorn, J. Haber, J. Gregoire, I. Sharp, **F. Toma**

11:00 CATL **383.** Investigating the structural dynamics of the Bi/$[BMIM]^+$ interface during electrocatalytic reduction of CO_2. **J. Medina Ramos**, S. Lee, A. Hubaud, T. Fister, P. Fenter

11:30 CATL **384.** Solvation and desolvation in nonaqueous zinc batteries. **T. Fister**, S. Kim, S. Han, K. Bassett, K. Ta, K.A. See, A. Gewirth, N. Rajput, K. Persson, P. Fenter

12:00 CATL **385.** MWCNTs/polyvinyl alcohol based flexible ethanol sensor: Density functional theory study of ethanol interactions at MWCNT-PVA interface. D. Maity, R. Krishnamoorthy, S. Lakshmipathi, **R. Rajendrakumar**

Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CATL and CEI

WEDNESDAY AFTERNOON

Section A

Walter E. Washington Convention Center
Room 101

Advances in Computational Catalysis

G. Mpourmpakis, R. Surendran Assary, *Organizers*

M. Dixit, D. Pahls, *Presiding*

1:00 Introductory Remarks.

1:05 CATL **386.** Adsorption free energies using neural network based potential energy sampling. **P. Mehta**, A. Lehmer, A. Bajpai, K. Frey, W.F. Schneider

1:25 CATL **387.** Computational study of the effect of surface-bound disulfide on the oxygen reduction reaction. **T.C. Allison**, Y. Tong

1:45 CATL **388.** Understanding heterogeneous catalyst deactivation by biogenic impurities on Ni (111) surface and bimetallic alloy. **M. Gupta**, T. Khan, S. Gupta, M. Alam, M. Agarwal, M. Haider

2:05 CATL **389.** Elucidating the role of heteronuclear interactions in boosting H_2 production from HCOOH decomposition on bimetallic Pd-M catalysts from first-principles. **J. Cho**, S. Lee, S. Yoon, J. Han, S. Nam, K. Lee, H. Ham

2:25 CATL **390.** SQERTSS for TPR: Dynamic throttling of lattice kinetic monte carlo to increase computational efficiency of spatial chemical kinetics simulations. J.E. Sutton, A. Beste, **A. Savara**, C. Hin, T. Danielson

2:45 Intermission.

3:00 CATL **391.** Effects of secondary coordination sphere of copper(III)-OH complexes on hydrogen atom transfer rates. **M. Momeni**, B. Dereli, D. Dhar, G. Yee, W.B. Tolman, C.J. Cramer

3:20 CATL **392.** Selective hydrogenation of acetylene on graphene supported single-atom Pt catalyst. **H. Zhuo**, X. Zhang, J. Li

3:40 CATL **393.** Kinetic Monte Carlo study of vinyl acetate synthesis from gas-phase ethylene acetoxylation on Pd(100) and Pd/Au(100) from density functional theory based calculations. **X. Dong**, Y. Huang, H. Jiang, Y. Yu, M. Zhang

4:00 CATL **394.** On the mechanism of CO_2 reduction to C2 products at copper surfaces. **A.J. Garza**, M.P. Head-Gordon, A.T. Bell

4:20 CATL **395.** Can copper be the active site in methanol synthesis? M. Shaban Tameh, A. Dearden, C. Huang

4:40 CATL **396.** Design of solid frustrated Lewis pair catalysts by surface oxygen vacancy regulation for hydrogenation reactions. **Z. Huang**, C. Chang

5:00 Concluding Remarks.

Section B

Walter E. Washington Convention Center
Room 102B

Vehicle Emission Control Catalysis: New Era, New Challenges & New Solutions

Cosponsored by ENFL and ENVR

F. Gao, C. H. Peden, *Organizers*, *Presiding*

1:00 CATL **397.** Methane oxidation over Pd containing catalysts for lean and stoichiometric conditions. N. Sadokhina, O. Mihai, G. Smedler, U. Nylén, M. Olofsson, **L. Olsson**

1:40 CATL **398.** Elucidating the chemical nature of a Pt single site catalyst supported on the '29' Cu surface oxide for low temperature CO oxidation. **R. Zhang**, A. Hensley, A. Therrien, K. Groden, A. Schilling, E.H. Sykes, J. McEwen

2:00 CATL **399.** Highly dispersed Pt-Pd bimetallic catalysts for diesel exhaust treatment. **A.P. Wong**, T. Toops, J.R. Regalbuto

2:20 Intermission.

2:40 CATL **400.** Multi-functional nanostructure array integration and manufacturing for emission control and utilization. **P. Gao**

3:00 CATL **401.** Regeneration of bimetallic Pt/Pd methane oxidation catalysts after sulfur exposure. **M.S. Wilburn**, W. Epling

3:20 CATL **402.** Cu-Co-Ce ternary oxide as an additive to conventional Pt/Al_2O_3 catalyst for lean exhaust catalysis. **A.J. Binder**, T. Toops, J. Parks

3:40 CATL **403.** Activity and stability of Co_3O_4-based catalysts for soot oxidation: The enhanced effect of Bi_2O_3 on activation and transfer of oxygen. W. Wang, C. Wang, **W. Li**, Y. Guo, Y. Guo, G. Lu

4:00 Concluding Remarks.

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

‡ *Cooperative Cosponsorship*

Section C

Walter E. Washington Convention Center
Room 102A

Advances in Carbon Dioxide Utilization

Cosponsored by ENFL and ENVR

F. Shi, *Organizer*

V. Abdelsayed, F. Jiao, *Organizers*, *Presiding*

1:00 CATL **404.** Photocatalytic reduction of CO_2 to CO over the UV-Vis-NIR spectrum on oxygen-deficient ZnO_{1-x}/carbon composites synthesized by aerosol routes. L. Lin, **S. Kavadiya**, Y. Nie, P. Biswas

1:20 CATL **405.** Photoreduction of CO_2 by SnO_2/graphene oxide composite particles. **Y. Liang**, W. Wu, D. Liu, S.H. Ehrman

1:40 CATL **406.** Facile development of MOFs-based nanocomposites for enhanced CO_2 photoreduction. **X. He**, D. Wang, W. Wang

2:00 CATL **407.** Converting CO_2 into fuels by graphitic carbon nitride based photocatalysts. **L. Zhang**

2:20 CATL **408.** Stable aqueous photoelectrochemical CO_2 reduction by a Cu_2O dark cathode with improved selectivity for carbonaceous products. **X. Chang**, T. Wang, J. Gong

2:40 Intermission.

2:55 CATL **409.** Withdrawn.

3:15 CATL **410.** Production of naphthalene from carbon dioxide and methanol by photocatalysis using nanostructured cobalt. **K. Davies**, D.K. Ryan

3:35 CATL **411.** Glycerol transfer hydrogenation of CO_2 using Ir and Ru carbene organometallics immobilized on hydrotalcites. **J. Heltzel**, M. Finn, A. Voutchkova

3:55 CATL **412.** Investigation of hydrogenation/disproportioation of formic acid to methanol using iridium catalysts. **Y. Himeda**, H. Kawanami, G. Laurenczy

Section D

Walter E. Washington Convention Center
Room 103B

Nanoporous Materials for Catalysis in Global Economy

E. Kyriakidou, Z. Li, D. Liu, H. Wang, *Organizers*, *Presiding*

1:00 Introductory Remarks.

1:05 CATL **413.** Catalytically functionalized nanoporous frameworks and carbons for chemical energy storage. **M. Allendorf**, J. Brown, J.L. White, V. Stavila, T. Heo, B. Wood, I. Klebanoff

1:40 CATL **414.** Computationally-driven design of cation-based catalysts supported in metal-organic frameworks for upgrading of light hydrocarbons. S.L. Pellizzeri, P. Miro, V. Bernales, M. Barona, P. Liao, L. Gagliardi, R. Snurr, **R. Getman**

2:05 CATL **415.** New modified nitrogen-doped graphene (N-G)/metal organic framework (MOF) derived microporous catalyst for oxygen reduction reaction (ORR). **S. Zhuang**, B. Nunna, E. Lee

2:30 CATL **416.** Withdrawn.

2:55 Intermission.

3:15 CATL **417.** Mesoporous manganese oxide catalyzed cross dehydrogenative coupling of *N*-arylletrahydroisoquinoles (sp^3 C-H) with indoles (sp^2 C-H). **B. Dutta**, S.L. Suib

3:40 CATL **418.** Study of the concentration enrichment effects in oxide nanotubes prepared by atomic layer deposition. **Z. Gao**, M. Wang, Y. Qin

4:05 Concluding Remarks.

Section E

Walter E. Washington Convention Center
Room 140A

New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics

B. Ginovska, M. J. O'Hagan, S. Raugei, *Organizers*

R. Koder, *Presiding*

1:00 CATL **419.** Novel supramolecular approach for multicatalytic activity of Mn-porphyrin derivative. **R. Kubota**, H. Kawakami

1:20 CATL **420.** Synthesis of hybrid catalysts and their application in alkane oxidation and CO_2 conversion. **A.J. Karkamkar**

1:45 CATL **421.** Assembly of bio-mimetic multienzyme complex on DNA nanoscaffolds. **J. Fu**

2:05 CATL **422.** Rational design of an artificial hydrogen peroxide oxidase and its use as an electron source for artificial reaction centers. **R.L. Koder**, S.D. Minteer, D.J. Vinyard, G.W. Brudvig, J. Preston, E. Andersen, B. Everson, E. Bjerkefeldt, F. Giroud

2:30 Intermission.

2:45 CATL **423.** Exploring peptoid nanomembranes as platform to mimic natural enzymes. **M.D. Baer**, C. Chen

3:10 CATL **424.** Enzyme inspired catalysts. **L. Connal**

3:30 CATL **425.** Role of anharmonicity in the confinement effect in zeolites: Structure, spectroscopy and adsorption free energy. M. Lee, Y. Wang, V. Glezakou, **R. Rousseau**

Section F

Walter E. Washington Convention Center
Room 140B

Multimodal Characterization of Functional Energy Materials

Advances *In Situ*/ Operando Microscopy

Cosponsored by ENFL

V. Murugesan, N. Rajput, L. Trahey, *Organizers*

S. Lakshmipathi, M. Nandasiri, *Presiding*

1:30 CATL **426.** *Operando* video microscopy of lithium metal anodes: From dendrite nucleation to cell failure. **N.P. Dasgupta**

2:00 CATL **427.** Correlating structure and electron transfer at nucleation sites on electrode surfaces. **K.L. Jungjohann**, S. Goriparti, W.M. Mook, G.A. Montano, M. Rush, K. Leung, K.R. Zavadil

2:30 CATL **428.** High-resolution characterization of intercalation cathodes for multi-valent battery applications. **R. Klie**, A. Mukherjee, J. Jokisaari, J.L. Andrews, H. Yoo, S. Banerjee, J. Cabana

3:00 CATL **429.** Understanding photocatalytic activity at the nanoscale using correlated electron and fluorescence microscopy. **M. Roeffaers**, E. Debroye, J. Van Loon

3:15 Intermission.

3:30 CATL **430.** Multi-modal approach to understand proton transport mechanisms in Y-doped barium zirconate. **R. Unocic**, J. Ding, J. Balachandran, X. Sang, W. Guo, J. Anchell, G. Veith, C.A. Bridges, Y. Cheng, C. Rouleau, J. Poplawsky, N. Bassiri-Gharb, P. Ganesh

4:00 CATL **431.** Decoding structure-property relationships of energy materials using atom probe tomography and correlative microscopy. **A. Devaraj**, E. Vo, P. Parikh, V. Murugesan, K.K. Ramasamy, S. Meng, C. Wang, S. Thevuthasan

4:30 CATL **432.** Modeling energy materials by integrating large microCT image volumes with data from microscopy, spectroscopy, and scattering. **D.Y. Parkinson**, I. Zenyuk, K. Harry, K. Higa, D. Devaux, N.P. Balsara, E. Gross

5:00 CATL **433.** Rectifying the characterization of carbon supported Pd: Chloride poisoning, carbon decoration, or both? R. Banerjee, J.R. Regalbuto

5:15 CATL **434.** Visible light driven photocatalytic properties of vertically aligned ZnO-CuS core-shell nanorod arrays: Importance of the coupling interface by the in situ generated ZnS shell layer. R. Kugalur Shanmugam, D. Ranjith Kumar, **R. Rajendrakumar**

Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CATL and CEI

WEDNESDAY EVENING

Electrochemical Technologies for Water Purification

Sponsored by ENVR, Cosponsored by CATL and CEI

Environmental Applications of Liquid Phase Catalysis for Green Chemical Processes of Renewable Materials

Sponsored by ENVR, Cosponsored by CATL and ENFL

Green Chemistry & the Environment

Sponsored by ENVR, Cosponsored by CATL and CEI

Heterogeneous Catalysis for Environmental & Energy Applications

Sponsored by ENVR, Cosponsored by CATL

Nano-Enabled Water Treatment Technologies: Applications & Implications

Sponsored by ENVR, Cosponsored by CATL

THURSDAY MORNING

Section A

Walter E. Washington Convention Center
Room 101

Catalytic Transformation of Renewable Plant Biomass to Enhance Global Economy

Cosponsored by ENFL

N. Yan, X. Zhang, *Organizers*, *Presiding*

8:00 CATL **435.** Adipic acid production from biomass-derivatived tetrahydrofuran-2,5-dicarboxylic acid via the combination of solid acids and iodide. **R. Balakumar**, M.J. Gilkey, D.G. Vlachos, B. Xu

8:20 CATL **436.** Mechanistic study of the catalytic dehydration of methyl lactate to acrylates over NaY and effect on selectivity control. **B.M. Murphy**, M.P. Letterio, J. Soreo, B. Xu

8:40 CATL **437.** Functionalized cellulose as fuel additive. **C. Xia**, M. Tu

9:00 CATL **438.** Reductive catalytic fractionation of lignocellulose: A lignin-first biorefinery. **T. Renders**, S. Van den Bosch, W. Schutyser, T. Vangeel, B.F. Sels

9:20 CATL **439.** Synthesis of glycerol carbonate from CO_2 and glycerol over CeO_2 catalysts: Effect of crystallite size of CeO_2 and reaction conditions. **L. Jiaxiong**, D. He

9:40 Intermission.

9:50 CATL **440.** Lowering the carbon foot print of the automobile industry through the in-mixing of modified biorefinery lignin for producing durable interior materials in cars. **J. Jiang**

10:10 CATL **441.** Precise deposition of Pt promoter onto silica supported cobalt for Fischer-Tropsch synthesis. **F. Almalki**, J. Monnier, J.R. Regalbuto

10:30 CATL **442.** Metal-free cleavage of C-O bonds via the combination of hydriodic acid and molecular H_2 in organic acid solvents. **M.J. Gilkey**, A.V. Mironenko, D.G. Vlachos, B. Xu

10:50 CATL **443.** Bio-terephthalic acid synthesis from cross metathesis of bio-sourced unsaturated carboxylic acids and consecutive one-pot cycloaddition and aromatization reactions. **E. Saraci**, L. Wang, K.H. Theopold, R.F. Lobo

11:10 CATL **444.** Enzymatic modification of resveratrol: Green strategies for *α*-glycosylation. **T. Marie**, G. Willig, A. Teixeira, A. Gratia, J. Renault, F. Allais

11:30 CATL **445.** Valorization of biomass derived lactones into fuels and chemicals. **M. Alam**, S. Gupta, A. Bohre, E. Ahmad, T. Khan, B. Saha, M. Haider

Section B

Walter E. Washington Convention Center
Room 102B

General Catalysis

D. Liang, R. Ma, A. B. Padmaperuma, *Organizers*

D. Liang, *Presiding*

8:00 CATL **446.** Characterization of iron contamination on equilibrium fluid catalytic cracking catalyst particles. **H. Jiang**, K.J. Livi, S. Kundu, W. Cheng

8:20 CATL **447.** Hot electron-driven photocatalytic water splitting. **B. Hou**, L. Shen, H. Shi, R. Kapadia, S. Cronin

8:40 CATL **448.** Photocatalytic degradation of methylene blue using vanadosilicate AM-6. **M. Ismail**, J. Mattheisen, E. Hishiya

9:00 CATL **449.** Enzyme Immobilization on magnetic nanoparticles for enhancing biocatalysis. **C. Liu**

9:20 CATL **450.** Fenton degradation of organic pollutions based on various nanocrystals/biomass composite loaded columns. **D. Liang**

9:40 Intermission.

9:55 CATL **451.** Layered double hydroxide supported gold nanoparticles towards lignin depolymerization. **Y. Song**, M. Crocker, K. Wilson, M. Isaacs, A.F. Lee

10:15 CATL **452.** Biocementation of soils through calcium carbonate precipitation using microbial catalysis. **R. Pinto Vilar**, T. Hoang, J. Alleman, B. Cetin, K. Ikuma

10:35 CATL **453.** TEMPO-oxidized cellulose nanocrystal/ RuCO nanoparticle composite as a catalyst for the reduction of 5-hydroxymethylfurfural to 2,5-dimethylfuran. **J. Zhang**, W. Xie, Q. Liang, Y. Ni

10:55 CATL **454.** Shape-selective FeMnK/Al_2O_3@Silicalite-2 core-shell catalyst for Fischer-Tropsch synthesis to lower olefins. **H. Wang**, S. Huang, Y. Wang, X. Ma

11:15 CATL **455.** Selective conversion of syngas into light olefins over a cobalt-zeolite bifunctional catalyst. **B. Maddi**, K.K. Ramasamy, M. Gray

Section C

Walter E. Washington Convention Center
Room 102A

General Catalysis

D. Liang, R. Ma, A. B. Padmaperuma, *Organizers*

A. J. Karkamkar, *Presiding*

8:00 CATL **456.** Preparation of high-surface-area active catalyst supports by atomic layer deposition. **T. Onn**, R.J. Gorte

8:20 CATL **457.** Fischer-Tropsch Synthesis over (Fe-Nb_2O_5)-based catalysts. **R.R. Soares**, W. Silva, M. Napolitano, U. Silva

8:40 CATL **458.** Synergetic catalysis by copper and iron in oxidation of reduced Keggin heteropolytungstates by dioxygen. **M. Kim**, M. Chamack, C.L. Hill, Y.V. Geletii

9:00 CATL **459.** Potential of nanostructured nonequilibrium catalysts for carbon nanomaterials and beyond. **M. Atwater**, L. Guevara, R. Welsh, B. Stone, A. Joy, E. Zurita-Torres

9:20 CATL **460.** Development of oxamides as general ligands for copper-catalyzed aminations. **J.F. Dropinski**

9:40 Intermission.

9:55 CATL **461.** Synthesis and mechanistic study of Pt-based Tri-metal catalysts for the ethanol oxidation reaction. **S. Jilani**, Y. Tong, D. Zager, E. Iyanobor

10:15 CATL **462.** Sustainable nanomaterials: Synthesis and applications in catalysis. **M. Gawande**, R.S. Varma, R. Zboril

10:35 CATL **463.** Computational and experimental characterisation of solvent effects in hydrogen cation catalysis of ethanol to diethyl ether. **M.S. Howard**, M.K. Ghosh, J.J. Leahy, S. Dooley

10:55 CATL **464.** Template based nanostructure MnO_{2-x} catalysts for the mild oxidation organic compounds. **A. Altaf**, A. Badshah, S. Kausar, S. Arshad

Section D

Walter E. Washington Convention Center
Room 103B

General Catalysis

D. Liang, A. B. Padmaperuma, *Organizers*

R. Ma, *Organizer, Presiding*

K. Lin, *Presiding*

8:00 CATL **465.** Withdrawn.

8:20 CATL **466.** Energetics of adsorbed formate and formic acid on Ni(111) by calorimetry. **W. Zhao**, S. Carey, S. Morgan, C.T. Campbell

8:40 CATL **467.** Unraveling structure sensitivity in phenol hydrogenaton on Pd nanostructures. **M. Haider**, S. Seshadri, S. Gupta, T. Khan, V. Prabhakaran

9:00 CATL **468.** Identification of suitable active sites for simultaneous conversion of alpha-MOB and beta-MEMOB into MMA and MAA. **J. Xu**, A. Lemonds

9:20 CATL **469.** Effect of aqueous and non-aqueous reaction media on hydrogenation of succinimide to 2-pyrrolidone. **S.R. More**, S.K. Tanielyan, R.L. Augustine, T. Thidarat, C. Ozmeral, K. Roffi, M. Shmorhun, J. Glas

9:40 Intermission.

9:55 CATL **470.** Characterization of Brønsted acid sites generated in situ on alkali-metal form zeolites via gas-solid ion exchange. **J. Soreo**, B.M. Murphy, B. Xu

10:15 CATL **471.** Withdrawn.

10:35 CATL **472.** Activation and stabilization of a silica-supported organochromium(III) complex resembling the union carbide catalyst. **Y. Wang**, X. Wang, B. Peters, S.L. Scott

Section E

Walter E. Washington Convention Center
Room 140A

General Catalysis

D. Liang, R. Ma, *Organizers*

A. B. Padmaperuma, *Organizer, Presiding*

A. Raju, *Presiding*

8:00 CATL **473.** New bidentate ligands for rhodium-catalysed branched selective propene hydroformylation. **L. Iu**, M. Janka, K.J. Fontenot, M.L. Clarke

8:20 CATL **474.** Withdrawn.

8:40 CATL **475.** C-C Bond cleavage of ethanol to form methane and carbon dioxide in liquid phase. **G. Yang**, X. Teng

9:00 CATL **476.** Constrained geometry organotitanium catalysts supported on nanosized silica for ethylene (co) polymerization. **K.T. Li**, L. Wu

9:20 CATL **477.** Description of adsorption processes by meta-generalized gradient approximations. **A.J. Garza**, A.T. Bell, M.P. Head-Gordon

9:40 Intermission.

9:55 CATL **478.** Determination of siting preference of exchanged Fe ions in Fe-SSZ-13 zeolite through density functional theory and ab Initio molecular dynamics. **S. Li**, W.F. Schneider

10:15 CATL **479.** In situ titration of carbon-supported electrocatalysts. **J. Egbert**, R.S. Weber

10:35 CATL **480.** Interaction of atomic oxygen with Ag(111) and Ag(110) surfaces: Oxygen adsorption and kinetics at surface versus subsurface. **S.B. Isbill**, S. Roy

10:55 CATL **481.** DNA-crowded enzyme complex with enhanced activity and stability. **J. Fu**

Section F

Walter E. Washington Convention Center
Room 140B

General Catalysis

D. Liang, R. Ma, A. B. Padmaperuma, *Organizers*

W. Wang, *Presiding*

8:00 CATL **482.** Plasmonic imaging technique for high throughput catalytic material screening. **X. Shan**, J. Chang

8:20 CATL **483.** Photocatalytic activity of sulfated TiO_2 and its application in water treatment. **S.F. Li**

8:40 CATL **484.** Novel sulfide based dehydrogenation catalysts. **P.H. Nielsen**, L.J. Lemus-Yegres, R.M. Nielsen

9:00 CATL **485.** Redox-auxiliary catalysis for cycling of photo-electro responsive materials. **S.C. Blackstock**, C. Nwankwoala, C. Saint-Louis, D. Warner, K. Strickland, L. Gray

9:20 CATL **486.** Mechanistic insights and new applications of palladium catalysts with multi-arylated phosphine ligands for cross-coupling. **H. Jong**, Y. Lim, S.T. Eey, W. Wu, C. Johannes, F. Yong, E.G. Robins, A.M. Mak, M.B. Sullivan

9:40 Intermission.

9:55 CATL **487.** CuI-catalyzed aerobic oxidation reaction of secondary alcohols promoted by a novel modified Cr-metal-organic framework ligand. **Y. Luan**, J. Zhao

10:15 CATL **488.** Enrichment at nano-interface for enhancing environmental catalytic oxidation. **W. Wang**

10:35 CATL **489.** Fundamental investigation of C-C coupling of carbonyl compounds on ceria. C. Zhao, A. Savara, **Y. Xu**

10:55 CATL **490.** Multicomponent Mannich reactions catalyzed by layered double hydroxide modified with copper. **Z. Wu**

Technical program information known at press time.
The official technical program for the 254th ACS National Meeting is available at www.acs.org/WDC2017

‡ *Cooperative Cosponsorship*

CELL

Division of Cellulose & Renewable Materials

M. Roman, *Program Chair*

SUNDAY MORNING

Section A

Grand Hyatt Washington
Penn Quarter A/B

Recent Advances towards the Bioeconomy

Cosponsored by AGFD, CARB, ENFL and ENVR

M. Roman, *Organizer*

D. Salas-de la Cruz, *Presiding*

8:00 Introductory Remarks.

8:05 CELL **1.** Rapid room temperature solubilization and depolymerization of polymeric lignin at high loadings. **J. Sun**, T. Dutta, N.G. Isern, J.R. Cort, B.A. Simmons, S. Singh

8:30 CELL **2.** Investigation of ionic liquid-lignin interactions and its effect on biomass pretreatment. **T. Dutta**, M. Valiev, X. Wang, N.G. Isern, J.R. Cort, B. Simmons, S. Singh

8:55 CELL **3.** Deep eutectic solvent fractionation of biomass. **M.B. Foston**

9:20 CELL **4.** Kinetic modeling of cellulose fractional pyrolysis. **H. Bennadji**, L. Khachatryan, S.M. Lomnicki

9:45 Intermission.

10:00 CELL **5.** Alkane production from biomass: A chemocatalytic liquid phase cellulose-to-naphtha process. **A. Deneyer**, M. Dusselier, B.F. Sels

10:25 CELL **6.** Catalytic dehydration of glucose and fructose into 5-hydroxymethylfurfural by aluminum complexes bearing bidentate (aminomethyl)phenolate ligands. **D.S. Saangonyo**, F.T. Ladipo

10:50 CELL **7.** Isolation and characterization of cellulose from biomass: Applications in biomedical and food packaging. N. Shahi, B. Min, D. Mortley, **V.K. Rangari**

11:15 CELL **8.** Cellulose nanocrystal production by sulfuric acid hydrolysis of wood pulp: What are reasonable yields? M. Roman, S. Dong, S. Welborn, S. Oxley, K. Chan, M.J. Bortner

11:40 Concluding Remarks.

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