

**2016 Catalysis Science PI Meeting
Science of Catalytic Reaction Mechanisms**

June 21-24, 2016

Marriott Washingtonian, Gaithersburg, MD

Program chairs: Tom Rauchfuss and Peter Stair

Tuesday Afternoon, June 21

2:00-5:00 p.m. **Registration**

Wednesday Morning, June 22

7:00-8:30 a.m. **Breakfast**

OPENING SESSION

Session Chairs: **Tom Rauchfuss and Peter Stair**

- 8:30-9:00 a.m. Welcoming remarks
Viviane Schwartz and Chuck Peden, DOE/BES/Catalysis Science Program
- 9:00-9:10 a.m. PI Meeting Theme – “*Science of Catalytic Reaction Mechanisms*”
Peter Stair, Northwestern Univ., **Tom Rauchfuss**, University of Illinois,
Champaign-Urbana
- 9:10-9:30 a.m. BES Update
Gail Mclean, DOE/BES/Chemical Sciences, Geosciences and Biosciences
Division

GENERAL SESSION I

Session Chair: **Peter Stair**, Northwestern University

- 9:30-10:10 a.m. Understanding and Controlling C-H Bond Transformations and Partial Oxidation of
Light Alkanes with Less and Less Oxygen
Eric McFarland, University of California, Santa Barbara
- 10:10-10:30 a.m. **Coffee Break**

GENERAL SESSION II

Session Chair: **Dan Mindiola**, University of Pennsylvania

- 10:30-11:10 a.m. Catalytic Approaches to Complex Molecules from Carbohydrate Biomass
Michel Gagne, University of North Carolina, Chapel Hill

- 11:10-11:40 a.m. Discovering Emergent Phenomena in Catalysis through Large Scale Ab Initio Molecular Dynamics Simulations
Roger Rousseau, Pacific Northwest National Laboratory
- 11:40-12:10 p.m. Oxidation Reactions on PdO(101)
Jason Weaver, University of Florida
- 12:10-1:30 p.m. **Working Lunch**

Wednesday Afternoon, June 22

GENERAL SESSION III

Session Chair: **Fabio Ribeiro**, Purdue University

- 1:30-2:10 p.m. Synthetic and Mechanistic Studies Pertaining to Homogeneous Catalytic Transformations of Small Molecules by Metal Centers
Ged Parkin, Columbia University
- 2:10-2:40 p.m. Analysis of the Mechanisms of Electrochemical Oxygen Reduction and Development of Ag-alloy and Pt-alloy Electro-catalysis for Low Temperature Fuel Cells
Suljo Linic, University of Michigan
- 2:40-3:10 p.m. Reaction Mechanisms of Oxygenates over Oxide Catalysts: Role of Surface Structure and Composition
Zili Wu, Oak Ridge National Laboratory
- 3:10-3:30 p.m. **Coffee Break**
- 3:30-5:00 p.m. **BREAKOUT SESSION I**
- 5:00-7:00 p.m. **Dinner (on your own)**

Wednesday Evening, June 22

- 7:00-9:00 p.m. **Posters (Odd numbers)**

Thursday Morning, June 23

7:00-8:00 a.m. **Breakfast**

GENERAL SESSION IV

Session Chair: **Peter Stair**, Northwestern University

8:00-8:50 a.m. **Breakout session I recap** (10 minutes each) – Breakout Session Chairs

8:50-9:30 a.m. Reaction Mechanisms: Interplay of Thermodynamics and Kinetics
Talat Rahman, University of Central Florida

9:30-10:00 a.m. Catalysis by Design: Heterogeneous Single Atom Catalysts
Maria Flytzani-Stephanopoulos, Tufts University

10:00-10:20 a.m. **Coffee Break**

GENERAL SESSION V

Session Chair: **Lars Grabow**, University of Houston

10:20-11:00 a.m. Towards More Accurate Descriptors of Reactivity in Acid and Oxidation
Catalysis on Metal Oxides
Enrique Iglesia, University of California, Berkeley

11:00-11:30 a.m. Electrocatalysis of Reactions for Direct Energy Conversion: Changing the
Reaction Mechanism for Increased Kinetics
Radoslav Adzic, Brookhaven National Laboratory

11:30-12:00 p.m. Highly Active Metal-Oxide Catalysts for Water Splitting
Aleksandra Vojvodic, SUNCAT/SLAC National Accelerator Laboratory

12:00-1:30 p.m. **Working Lunch**

Thursday Afternoon, June 23

1:30-3:00 p.m. **BREAKOUT SESSION II**

3:00-3:20 p.m. **Coffee Break**

PLENARY SESSION

Session Chair: **Tom Rauchfuss**, University of Illinois, Champaign-Urbana

- 3:20-4:20 p.m. Hydrocarbon Conversions Catalyzed by Iridium Complexes: High and Low Oxidation States
Invited lecture – Alan Goldman, Rutgers University
- 4:20-4:50 p.m. Mechanistic Studies of Bioinspired Oxidative Organometallic Reactions
Liviu Mirica, Washington University
- 4:50-7:00 p.m. **Dinner (on your own)**

Thursday Evening, June 23

- 7:00-9:00 p.m. **Posters (Even numbers)**

Friday Morning, June 24

- 7:00-8:00 a.m. **Breakfast**

GENERAL SESSION VI

Session Chair: **Bill Jones**, University of Rochester

- 8:00-8:40 a.m. The Interconversion of Ammonia with Its Elements
Paul Chirik, Princeton University
- 8:40-9:10 a.m. Molecular-Level Design of Heterogeneous Chiral Catalysts
Eddy Tysoe, University of Wisconsin, Milwaukee
- 9:10-9:40 a.m. Organometallic Chemistry for Alkane Dehydrogenation
Adam Hock, Illinois Institute of Technology and Argonne National Lab
- 9:40-10:20 a.m. Stereospecific ROMP of Cyclic Olefins with Mo and W Initiators
Richard Schrock, Massachusetts Institute of Technology
- 10:20-10:40 a.m. **Coffee Break**

CLOSING SESSION

Session Chair: **Tom Rauchfuss**, University of Illinois, Champaign-Urbana

- 10:40-11:40 a.m. **Breakout session II recap** (15 minutes each) – Breakout Session Chairs
- 11:40-12:00 p.m. Closing Remarks
Rauchfuss, Stair, Schwartz, Peden
- 12:00 p.m. **Adjourn**