

# “Mechanistic Homogeneous Catalysis - A Meeting between Theory and Experiment”

Wenner-Gren Center, Stockholm, September 4-7, 2019

**Organizing committee:** Fahmi Himo and Kalman Szabo  
**Secretariat Wenner-Gren Foundations:** Maria Helgöstm

## Wednesday, September 4<sup>th</sup>

**18.00-20.30 Registration and Welcome reception with buffet dinner**

## Thursday, September 5<sup>th</sup>

8.00-8.45 Registration and coffee

8.45-8.55 Welcome address: Britt-Marie Sjöberg, Wenner-Gren Foundations

8.55-9.00 Introduction: Kalman Szabo

### Session I. Chair: Kalman Szabo

9.00-9.40 **Eiichi Nakamura**, University of Tokyo, Japan

*“Molecular electron microscopy for studies on mechanism of molecular motions and reactions”*

**9.40-10.10 Coffee break**

10.10-10.50 **Feliu Maseras**, Institute of Chemical Research of Catalonia, Spain

*“From free energy profiles to reaction times through microkinetic modeling”*

10.50-11.30 **Jason Hein**, University of British Columbia, Canada

*“The secret lives of Cu(I)-Acetylides”*

**11.30-11.40 Leg stretcher**

11.40-12.20 **Jeremy Harvey**, KU Leuven, Belgium

*“Deconstructing reaction mechanisms in silico: how far can we go?”*

**12.20-13.30 Lunch**

**Session II. Chair: Francisco Juliá-Hernández**

13.30-14.10 **Jan-Erling Bäckvall**, Stockholm University, Sweden  
*“Mechanistic studies of iron- and palladium-catalyzed reactions of allenes”*

14.10-14.50 **Edward Anderson**, Oxford University, UK  
*“Combining experiment with theory in transition metal-catalyzed reactions of strained rings”*

**14.50-15.00 Leg stretcher**

15.00-15.40 **Rob Paton**, Colorado State University, USA  
*“New modes of organic reactivity and enantioselectivity from modeling and informatics approaches”*

**15.40-16.10 Coffee break**

16.10-16.50 **Laurence Grimaud**, Sorbonne University, France  
*“Boron to transition metal transmetalation: from mechanistic studies to rational development”*

16.50-17.30 **Sason Shaik**, Hebrew University, Israel  
*“Oriented-external-electric-fields - new effectors in chemistry”*

**17.45-22.00 Boat trip and dinner**

**Friday, September 6<sup>th</sup>**

**Session III. Chair: Nicklas Selander**

08.30-9.10 **Paul Chirik**, Princeton University, USA  
*“Catalysis with earth abundant metals: new mechanisms and applications to organic synthesis”*

9.10-9.50 **Vidar Jensen**, University of Bergen, Norway  
*“The life, death, and resurrection of ruthenium olefin metathesis catalysts”*

**9.50-10.15 Coffee break**

10.15-10.55 **Peng Liu**, University of Pittsburgh, USA  
*“Predictive models for transition metal-catalyzed organic reactions”*

10.55-11.35 **Licheng Sun**, KTH Royal Institute of Technology, Sweden  
*“Water splitting in nature and man-made systems: mechanisms of O-O bond formation”*

**11.35-11.45 Leg stretcher**

11.45-12.25 **James Mayer**, Yale University, USA  
*“Proton-coupled electron transfer in homogeneous catalysis”*

**12.25-13.30 Lunch**

**Session IV. Chair: Abraham Mendoza**

13.30-14.10 **Odile Eisenstein**, University of Montpellier, France

*“The <sup>13</sup>C solid state NMR signature of metal-bonded carbon: an information for bonding and reactivity”*

14.10-14.50 **Kazushi Mashima**, Osaka University, Japan

*“Approach to generate new catalytically active species based on reaction mechanism”*

**14.50-15.00 Leg stretcher**

15.00-15.40 **Paolo Melchiorre**, Institute of Chemical Research of Catalonia, Spain

*“The photochemistry of organocatalysis – a mechanistic perspective”*

15.40-16.20 **Paul Zimmerman**, University of Michigan, USA

*“Tracking the electronic and structural changes of transition metals in new catalysis methods”*

**16.20-16.50 Coffee break**

16.50-17.30 **Zhenyang Lin**, The Hong Kong University of Science and Technology

*“Boryls, their metal complexes, and catalysis: theoretical and computational insights”*

17.30-18.10 **Agustí Lledos**, Autonomous University of Barcelona, Spain

*“From organometallics to artificial metalloenzymes: Cu-catalyzed enantioselective hydration of alkenes”*

**18.30-22.00 Vasa museum and dinner**

**Saturday, September 7<sup>th</sup>**

**Session V. Chair: Fahmi Himo**

9.00-9.40 **Kendall Houk**, University of California Los Angeles, USA

*“Computational explorations of organo- and transition metal-catalyzed reactions”*

9.40-10.20 **Scott Denmark**, University of Illinois, USA

*“Prediction of higher-selectivity catalysts by computer-driven workflow and machine learning”*

**10.20-10.50 Coffee break**

10.50-11.30 **Dean Toste**, University of California Berkeley, USA

*“Homogeneous catalysis in confined spaces”*

11.30-12.10 **Julius Rebek**, The Scripps Research Institute, USA

*“Chemistry of confined molecules”*

**12.10-12.30 Discussion and Conclusions**

**12.30 -13.30 Lunch**