International Conference on Theoretical Aspects of Catalysis

June 24 - 28, 2018. UCLA campus, Los Angeles, California, USA

Sponsors:

UCLA Chemistry & Biochemistry

nature catalysis

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ACS Catalysis

International Conference

on Theoretical Aspects of Catalysis (ICTAC)

Technical Program

invited talks, contributed talks

Sunday, June 24

Arrival and registration. Registration begins at 3:30 pm. UCLA Faculty Center.

Afternoon:
Welcoming remarks – Philippe and Anastassia

4:00 – 4:40 pm Emily Carter (Princeton University)
"Mechanisms for Sustainable Fuel and Chemical Production from First Principles"

4:40 – 5:20 pm Robert Morris (University of Toronto)
"Catalytic Asymmetric Hydrogenation: Practice and Theory"

5:20 – 7 pm Conference Reception

Monday, June 25

Doors open at 8:30 am

Morning: Electrocatalysis *Presiding: Romain Reocreux*

9:00 – 9:40 am Jan Rossmeisll (University of Copenhagen)
"Modelling the Electrochemical Interface - Ions Influence on Electrocatalysis"

9:40 – 10:00 am Tao Cheng (Caltech)
"Active Sites for Promoting Carbon Dioxide Reduction on Metal Nanoparticles: Atomic-scale Insights from Multiscale Simulations"

10:00 – 10:20 am Cody Finke (Caltech)
"Enhancing oxygen and chlorine evolution electrocatalytic activity by atomic layer deposition"

10:20 – 10:40 am Coffee Break

10:40 – 11:00 am Yousung Jung (KAIST)
"Electrochemical activation of small molecules using electronic structure calculations and machine learning approaches"

11:00 – 11:20 am Megha Anand (Stanford University)
"Oxygen Reduction Reaction on Metal Porphycenes adsorbed on Au(111) surface"

11:20 – 11:40 am Yuemei Zhang (University of California, Riverside)
"Density Functional Theory Inverstigations on the Catalytic Activity of Metal Diborides for Hydrogen Evolution"

11:40 – 12:00 pm Ambuj Tiwari (University of Amsterdam and Amsterdam Center for Multiscale Modeling)
"Proton coupled electron transfer reactions at $RuO_2(110)$ - water interface"

12:00 – 1:00 pm Lunch

Afternoon:

1:00 – 2:30 pm Poster Session

Homogeneous Catalysis *Presiding: Ye Xu*

2:30 – 3:10 pm Christopher Cramer (University of Minnesota)
"Spiral Feedback for Catalyst Design: Experiment and Theory"

3:!0 – 3:50 pm Lynn Kamerlin (Uppsala University)
"Conformational Dynamics and the Evolution of New Enzyme Functions"

3:50 – 4:10 pm Coffee Break

4:10 – 4:30 pm Matthew Wodrich (Ecole Polytechnique Fédérale de Lausanne)
"Identifying Highly Active and Regioselective Homogeneous Catalysts from Molecular Volcano Plots"

4:30 – 4:50 pm Vidar Jensen (University of Bergen)
"Automated in Silico Design of Homogeneous Catalysts"

4:50 – 5:10 pm Robert Froese (The Dow Chemical Company)
"Theoretical Studies of Rhodium Catalyzed Hydroformylation of Olefins"

5:10 – 5:30 pm Raphael Wischert (CNRS-Solvay)
"Direct Amination of Alcohols Catalyzed by Aluminium Triflate: an Experimental and Computational Study"

Dinner on own

Tuesday, June 26

Doors open at 8:45 am

Morning: Heterogeneous Catalysis *Presiding: Borna Zandkarimi*

9:00 – 9:40 am William Goddard (Caltech)
"Quantum Mechanics based reaction mechanisms for Catalysts"

9:40 – 10:00 am Fanglin Che (University of Toronto)
"Methane Steam Reforming: Using External Electric Fields to Enhance the Catalytic Performance of Ni-based Catalysts"

10:00 – 10:20 am Runhong Huang (University of California, Riverside)
"Understanding the direct conversion of bio-ethanol to propene on In_2O_3 from first-principles calculations"

10:20 – 10:40 am Coffee Break

10:40 – 11:00 am Aravand Asthagiri (The Ohio State University)
"Low Temperature Selective Alkane Activation on IrO_2(110) Surfaces"

11:00 – 11:20 am Julia Schumann (Stanford University and SLAC)
"The Cu/ZnO methanol synthesis catalyst – insights from theory"

11:20 – 11:40 am Francesc Viñes (University of Barcelona)
"CO2 Capture and Conversion Using Transition Metal Carbide Systems"

11:40 – 12:00 pm Matthew Quesne (Cardiff University)
"Bulk and surface properties of metal carbides: implications for catalysis"

12:00 – 1:00 pm Lunch

Afternoon:

1:00 – 2:30 pm **Poster Session**

Solvation *Presiding: Kaining Duanmu*

2:30 – 3:10 pm Hans-Joachim Freund (Fritz-Haber Institute of the MPG)
"The Structure of Oxide Surfaces and its Interaction with Water"

3:10 – 3:30 pm Romain Réocreux (University College London)
"How to make γ-Al_2O_3 water-resistant ? Ab Initio Metadynamics at a solid/liquid interface."

3:30 –3:50 pm *Coffee Break*

3:50 – 4:30 pm Carine Michel (Ecole Normale Supérieure de Lyon, CNRS)
"Modeling reactivity at the solid/liquid interface: are we there yet?"

4:30 – 4:50 pm Rachel Getman (Clemson University)
"Molecular-Level Insights into How the Structure of Liquid Water Influences the Catalysis of Sugar Alcohol Conversions"

4:50 – 5:10 pm Evert Jan Meijer (University of Amsterdam)
"Novel Insights in the Role of Solvent in Catalytic Processes"

5:10 – 6:00 pm **Meet Your Editors** - Forum with Joachim Sauer (J. Catal.), Marcal Capdevila-Cortada (Nat. Catal.), Philippe Sautet (ACS Catal.)

6:00 – 7:00 pm **Drinks with your Editors – event sponsored by Elsevier**

Dinner on own

Wednesday, June 27

Doors open at 8:45 am

Morning: Kinetic simulations *Presiding: Anastassia Alexandrova*

9:00 – 9:40 am Michail Stamatakis (University College London)
"Understanding and Harnessing the "Odd One Out": Designing Single Atom Alloy Materials for Catalysis"

9:40 – 10:00 am Aditya "Ashi" Savara (Oak Ridge National Laboratory)
"Kinetic Simulations of Catalysis: From Multiple Surfaces to Physical Mixtures"

10:00 – 10:20 am Martin Hangaard Hansen (Stanford University)
"Micro-kinetic Modeling and Trends in Catalytic Dehydrogenation of Ethane"

10:20 – 10:40 am *Coffee Break*

Biocatalysis

10:40 – 11:20 am Steven Boxer (Stanford University)
"Electric Fields and Enzyme Catalysis"

11:20 – 11:40 am Valerie Vaissier Welborn (University of California, Berkeley)
"Enzyme design via electric field optimization"

11:40 – 12:00 pm David Reilley (University of California, Los Angeles)
"Capturing and designing for electrostatic preorganization in enzymes"

12:00 – 1:00 pm *Lunch*

Afternoon:
1:00 – 2:30 pm Poster Session

Catalysis by Clusters and Atoms *Presiding: Rachel Getman*

2:30 – 3:10 pm Jun Li (Tsinghua University)
"From Nanocatalysis to Dynamic Single-Atom Catalysis (DSAC)"

3:10 – 3:30 pm Andreas Heyden (University of South Carolina)
"Identifying Active Sites of the Water-Gas Shift Reaction over Titania Supported Platinum Catalysts under Uncertainty"

3:30 –3:50 pm Coffee Break

3:50 – 4:30 pm Stefano Fabris (Istituto Officina dei Materiali)
"Modeling the Effects of Chemical Enviornments on Oxide-Supported Catalysts"

4:30 – 4:50 pm Huanchen Zhai and Borna Zandkarimi (University of California, Los Angeles)
"Surface-Supported Cluster Catalysts: Fluxionality and Statistical Ensemble Nature"

4:50 – 5:10 pm Geng Sun (University of California, Los Angeles)
"Meta-stable structures in cluster catalysis from first-principles: Structural ensemble in reaction conditions and meta-stability triggered reactivity"

5:10 – 5:30 pm Manuel Louwerse (Utrecht University)
"Mechanisms for metal ion diffusion over hydroxylated support surfaces"

Dinner on own

Thursday, June 28

Doors open at 8:45 am

Morning: MOFs and Zeolites *Presiding: Philippe Sautet*

9:00 – 9:40 am Laura Gagliardi (University of Minnesota)
"Computationally Guided Discovery of Metal-Decorated Metal–Organic Frameworks Active for Catalysis"

9:40 – 10:00 am Maristella Alessio (Humboldt University of Berlin)
"Hybrid QM:QM Methods for Extended Periodic Systems"

10:00 – 10:20 am Dorothee Berthomieu (Institut Charles Gerhardt Montpellier and CNRS, ENSCM)
"Metal Coordination in Cu(II)-SSZ-13 Exposed to NH_3: DFT with in situ XAS experiment studies"

10:20 –10:40 am Coffee Break

10:40 – 11:00 am Roderigh Rohling (Eindhoven University of Technology)
"Detailed electronic structure analysis of the Diels-Alder cycloaddition between 2,5-dimethylfuran and ethylene over transition metal exchanged faujasites"

11:00 – 11:20 am Philipp Plessow (Karlsruhe Institute of Technology)
"Modeling the Kinetics of the Initiation of the MTO Process using ab-initio and DFT-calculations"

11:20 – 11:40 am Maciej Gierada (Cracow University of Technology)
"Modelling of CrO_x/SiO_2 and WO_x/SiO_2 *catalysts - formation of active sites for ethylene polymerization and propene metathesis"*

11:40 am – 12:00 pm Wilke Dononelli (Carl von Ossietzky University Oldenburg)
"A combined DFT and CCSD(T) study about oxygen activation and methanol oxidation on coinage metal catalysts"

12:00 pm – Closure by Anastassia & Philippe, and meeting adjourn