

4th Challenges in Computational Homogeneous Catalysis

Näsby Slott – Stockholm

14-16 June 2017

Wednesday 14 June

Arrival during the day

19.00 – Dinner

Thursday 15 June

Session I: (Chair: Fahmi Himo)

08.45 – 09.00 Conference Opening

09.00 – 09.30 Michele Parrinello

Fluctuations, Entropy and Rare Events

09.30 – 10.00 Christopher Cramer

Continuum Solvation - Powers and Pitfalls

10.00 – 10.30 Michelle Coote

Challenges for Modelling Electrostatic Catalysis of Non-Electrochemical Reactions

10.30 – 11.00 Coffee Break

Session II: (Chair: Nurcan Tüzün)

11.00 – 11.30 Gregori Ujaque

Dealing with Water in Au-Catalyzed Hydration of Unsaturated Compounds

11.30 – 12.00 Evert Jan Meijer

Multiple Pathways in Solvent-Mediated Chemical Reactions

12.00 – 12.30 Thibault Cantat

Does CO₂ Bending and Activation by a Frustrated Lewis Pair Facilitate its Reduction by Hydride Transfer?

12.30 – 13.00 Paul Zimmerman

Targeting Catalytic Chemistry at Covalent Bonds: Local Representations of Reactions and Electronic Correlations

13.00 – 14.30 Lunch

Session III: (Chair: Nino Russo)

- 14.30 – 15.00 Wei-Hai Fang**
Inert-Bond Functionalization by Visible Light Photoredox Catalysis with Ruthenium or Iridium Complexes
- 15.00 – 15.30 Henrik Ottosson**
Putting Baird's Rule on Excited State Aromaticity and Antiaromaticity into Action
- 15.30 – 16.00 Bo Durbeej**
Making Molecular Motors Rotate Faster
- 16.00 – 16.30 Laura Gagliardi**
Multireference Methods for Catalysis

16.30 – Coffee

19.00 – Dinner

Friday 16 June

Session IV: (Chair: Şaron Çatak)

- 09.00 – 09.30 Odile Eisenstein**
Have Carbon-13 NMR Chemical Shifts Predictive Power in Metathesis?
- 09.30 – 10.00 Feliu Maseras**
Concentration Effects are Absent from the (Usual) Free Energy Profiles
- 10.00 – 10.30 Marcin Kalek**
Analysis of Selectivity in Synergistic Catalysis by Means of Combined DFT Calculations and Kinetics Simulations

10.30 – 11.00 Coffee Break

Session V: (Chair: Ivan Rivalta)

- 11.00 – 11.30 Jamal Musaev**
Mono-N-Protected Amino Acid Ligand and Predictive Enantioselectivity Model for Pd-Catalyzed C-H Functionalization
- 11.30 – 12.00 Eric Clot**
DFT Studies of Pd-Catalyzed Enantioselective C-H Functionalization Processes
- 12.00 – 12.30 Miho Hatanaka**
Global Reaction Route Mapping Study on Asymmetric C-C Bond Formation

12.30 – 14.00 Lunch

Session VI: (Chair: Maria Ramos)

14.00 – 14.30 Agustí Lledós

The Multifaceted Reactivity of Late Transition Metal-Active Oxygen Complexes with Organic Substrates

14.30 – 15.00 Robert Paton

Chiral Counterions in Homogeneous Catalysis

15.00 – 15.30 Rong-Zhen Liao

Challenges in Modeling Water Oxidation Reactions

15.30 – 16.00 Jeremy Harvey

Understanding Catalysis with Non-Noble Metals: Free Energy as a Guide to Mechanism

16.00 – Conference Closing and Coffee

19.00 – Conference Dinner

Saturday 17 June

08.00 – 09.00 Breakfast

– 12.00 Departure