3rd Challenges in Computational Homogeneous Catalysis

Lovik - Stockholm
3-4 Sept 2015

Thursday 3 Sept

Session I: ***(Chair: Fahmi Himo)***

09.00 – 09.10 Conference Opening

09.10 – 09.45 Keiji Morokuma
The Global Reaction Route Mapping (GRRM) Strategy and Its Applications to Organometallic and Organic Catalysts.

09.45 – 10.20 Clemence Corminboeuf
Putting Forward Replica Exchange Molecular Dynamics and Other New Tools for Computational Homogenous Catalysis

10.20 – 10.55 Feliu Maseras,
Not Everything is in the Transition State

10.55 – 11.20 Coffee Break

Session II: ***(Chair: Bo Durbeej)***

11.20 – 11.55 Daniel Singleton
Controlling Selectivity by Controlling the Path of Trajectories

11.55 – 12.30 Gregori Ujaque
AIMD Applications to Organometallic Reactivity

12.30 – 13.05 Evert Jan Meijer
Insight into the Role of Solvents in Chemical Reactivity

13.05 – 13.30 Timofei Privalov
Molecular Motions and Chemical Reactivity - The Case of Frustrated Lewis Pairs

13.30 – 14.45 Lunch

Session III: ***(Chair: Vicente Moliner)***

14.45 – 15.20 Per Siegbahn
Similarities and Differences in Modeling Natural and Artificial Water Oxidation

15.20 – 15.55 Laura Gagliardi
Challenges in the Theoretical Characterization of Metal-Metal Containing Species as Catalysts for Small Molecule Activation

15.55 – 16.30 Zhenyang Lin
Computational Insight into Mechanism of Nickel-Catalyzed Reductive Carboxylation of Styrenes Using Carbon Dioxide

16.30 – 16.55 Mårten Ahlquist
C-H Activation by Ir complexes - Using Theory to Explain Ambiguous Experimental Observations

16.55 – 17.20 Coffee Break

Session IV: ***(Chair: Per-Ola Norrby)***

17.20 – 17.55 **Veronique Van Speybroeck**
First-Principle Modeling of Chemical and Physical Transformations in Complex Molecular Environments
17.55 – 18.30 **Satoshi Maeda**
Development of the Global Reaction Route Mapping Strategy for Catalysis
18.30 – 19.05 **Vidar Jensen**
Artificial Evolution of Homogeneous Catalysts

19.30 – **Dinner**

Friday 4 Sept

Session V: ***(Chair: Jan-Erling Bäckvall)***

09.00 – 09.35 **Kendall Houk**
Elucidation of Mechanisms and Selectivities of Catalytic Reactions
09.35 – 10.10 **Raghavan Sunoj**
Synergizing Theory and Experiments in Asymmetric Catalysis through Transition State Modeling: Leads for Rational Catalyst Design
10.10 – 10.45 **Agustí Lledós**
Computational Homogeneous Catalysis: More than Calculating Energy Profiles

10.45 – 11.10 **Coffee Break**

Session VI: ***(Chair: Pher Andersson)***

11.10 – 11.45 **Jeremy Harvey**
Reaction Mechanisms in Solution: Attempts to Build Accurate Models
11.45 – 12.20 **Franziska Schoenebeck**
On the Role of Dispersion in Organometallic Reactivity
12.20 – 12.55 **Olaf Wiest**
Computational Studies of Selectivity in Transition Metal Catalyzed Reactions
12.55 – 13.20 **Fahmi Himo**
Modeling of Water-Soluble Capsules

13.20 – 14.30 **Lunch**

Session VII: ***(Chair: Marcus Lundberg)***

14.30 – 15.05 **Stuart MacGregor**
Towards Computational Modelling of Organometallic Structure and Reactivity in the Solid State
15.05 – 15.40 **Christopher Cramer**
Exploiting the Metal-Organic Frameworks NU-1000 and UiO-6n for Catalysis at the Homogeneous/Heterogeneous Interface
15.40 – 16.15 **Odile Eisenstein**
Learning from Calculating NMR Chemical Shifts

16.15 – **Conference Closing**
20.00 – ***Conference Dinner at Tabbouli Restaurant***