Program

Thursday 25 Aug

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

09.00 – 09.35 **Feliu Maseras**, Institute of Chemical Research of Catalonia, Spain
Conformational complexity: a hidden price in the calculation of larger systems
09.35 – 10.10 **Sason Shaik**, Hebrew University, Israel
The Valence Bond Way in Bioinorganic Chemistry
10.10 – 10.45 **Jan-Erling Bäckvall**, Stockholm University, Sweden
Mechanistic Studies on Racemization of Alcohols Catalyzed by Cyclopentadienyl Ruthenium Complexes

10.45 – 11.05 Coffee Break

Session II: ***(Chair: Filippo De Angelis)***

11.05 – 11.40 **Vidar Jensen**, University of Bergen, Norway
Darwinian Optimization of Homogeneous Catalysts
11.40 – 12.15 **Natalie Fey**, University of Bristol, UK
Ligand Effects on Catalytic Cycles
12.15 – 12.50 **Sebastian Kozuch**, Weizmann Institute, Israel
What Makes for a Good Catalytic Cycle? Insights from the Energetic Span Model

13.00 – 14.30 Lunch

Session III: ***(Chair: Björn Åkermark)***

14.30 – 15.05 **Peter Comba**, University of Heidelberg, Germany
Mechanistic Aspects of the Activation of Dioxygen by High-Valent Iron Complexes
15.05 – 15.40 **Per Siegbahn**, Stockholm University, Sweden
Comparison of Natural and Artificial Water Oxidation
15.40 – 16.00 **Ivan Rivalta**, Yale University, USA
Computational Studies of Natural and Artificial Photosynthesis
16.00 – 16.20 **Lubomir Rulisek**, Czech Academy of Sciences, Czech Republic
En Route from Insight to Quantitative Accuracy in Theoretical Studies of Catalyzed Reactions

16.20 – 16.50 Coffee Break

Session IV: ***(Chair: Pedro Fernandes)***

16.50 – 17.25 **Gregori Ujaque**, Autonomous University of Barcelona, Spain
Modelling Homogeneous Catalysis in Water
17.25 – 18.00 **Filippo De Angelis**, ISTM-CNR Perugia, Italy
Ab Initio Molecular Dynamics Simulations of Organometallic Reactivity
18.00 – 18.35 **Xin Xu**, Fudan University, China
Computational Homogenous Catalysis: Gas Phase Values Plus Solvation Energies

19.00 – Buffet Dinner at Stora Skuggan

Friday 26 Aug

Session V: ***(Chair: Tore Brinck)***

09.00 – 09.35 **Imre Papai**, Hungarian Academy of Sciences, Hungary
Catalytic Hydrogenation with Frustrated Lewis Pairs
09.35 – 10.10 **Emilia Sicilia**, University of Calabria, Italy
Catalytic Generation of Hydrogen: Theoretical Study of Useful Hydrogen Storage Materials
10.10 – 10.30 **Timofei Privalov**, Stockholm University, Sweden
Inorganic Reaction Mechanisms and Catalysis of Proton Coupled Atom Transfer

10.30 – 11.00 Coffee Break

Session VI: ***(Chair: Ulf Wahlgren)***

11.00 – 11.35 **Michael Buehl**, University of St Andrews, UK
Computational Gold Catalysis
11.35 – 11.55 **Mårten Ahlquist**, Royal Institute of Technology, Sweden
Reactivity of Au-C Bonds towards Electrophilic Reagents
11.55 – 12.30 **Laurent Maron**, University of Toulouse, France
Determination of Activation Barrier of Bond Activation by d^0 Complexes
12.30 – 12.50 **Tommaso Marcelli**, Politecnico di Milano, Italy
Boronic Acid-Catalyzed Amide Bond Formation: Insights from DFT Calculations

13.00 – 14.30 Lunch

Session VII: ***(Chair: Hans Adolfsson)***

14.30 – 15.05 **Per-Ola Norrby**, University of Gothenburg, Sweden
Selectivities in Homogeneous Catalysis
15.05 – 15.40 **Eric Clot**, University of Montpellier, France
On the Use of Dispersion Corrections in Computational Studies of Transition Metal Reactivity
15.40 – 16.00 **Fahmi Himo**, Stockholm University, Sweden
Some Examples of Dispersion Effects on Selectivities
16.00 – 16.35 **Luigi Cavallo**, University of Salerno, Italy
Flexible Transition States and Dispersion Interactions; Two Challenges in the Modeling of Reactions in the Homogeneous Phase.

16.35 – Conference Closing

19.00 – 22.00 Conference Dinner on board S/S Stockholm to the Stockholm archipelago