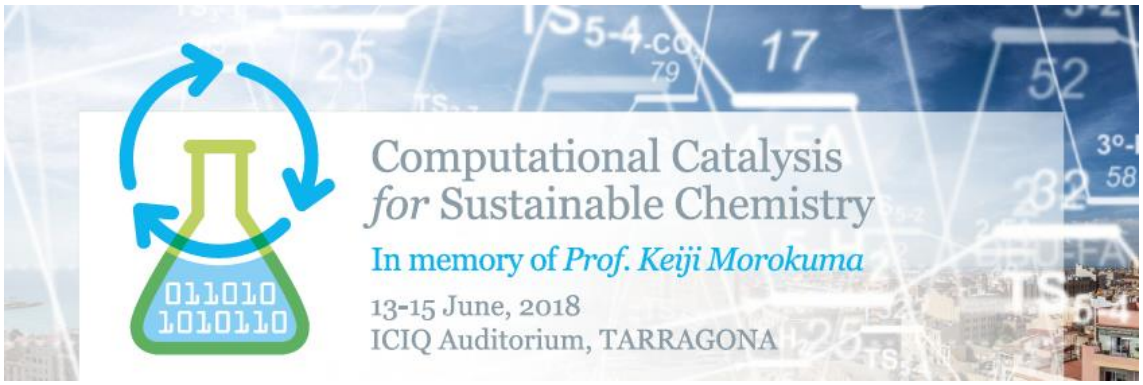


PROGRAMME

Wednesday, 13th June

11:50 – 14:15 Registration

14:15 – 14:30 Opening Ceremony

14:30 – 15:05 Walter Thiel
Computational Studies of Transition Metal Catalysis and Biocatalysis

15:05 – 15:40 Satoshi Maeda
Artificial Force Induced Reaction Method: Its Implementation and Development

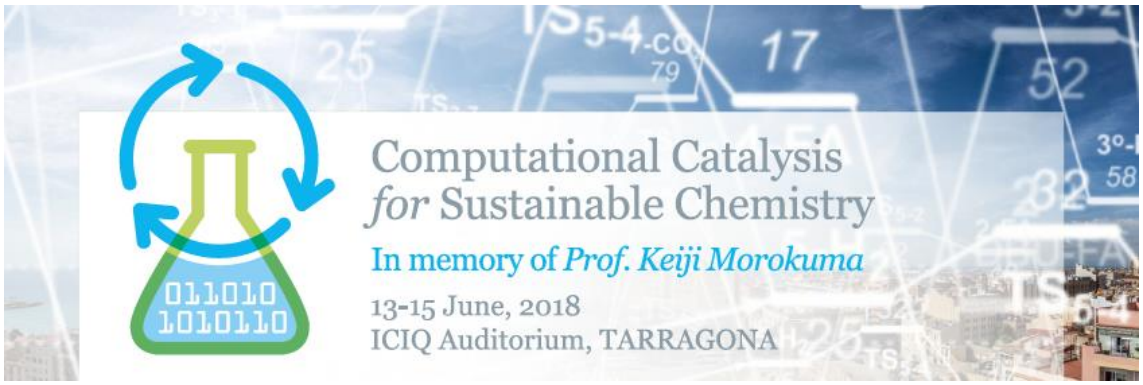
15:40 – 16:15 Kathrin Hopmann
Selectivity!

16:15 – 16:50 Luigi Cavallo
Tuning Proximal and Remote Steric Effects in the Rationalization of Catalytic Behavior

16:50 – 17:15 Coffee Break

17:15 – 17:50 Philippe Sautet
Crucial role of metastable structures of Pt clusters for light alkane activation

17:50 – 18:25 Maria Besora
What are Bond Dissociation Energies made out of?



Thursday, 14th June

9:00 – 9:35 Joachim Sauer
Computational Catalysis – Rigor and Relevance

9:35 – 10:10 Miho Hatanaka
Application of Automated Reaction Path Search Method to a Systematic Search of Transition States: A Case Study on Asymmetric Catalytic Reaction

10:10 – 10:45 Lionel Perrin
When Computational Chemistry Meets Experiments in Polymerization Catalysis

10:45 – 11:15 Coffee Break

11:15 – 11:50 Maria Joao Ramos
Understanding enzymes. Can we accurately predict mechanisms of enzymatic reactions?

11:50 – 12:25 Rob Paton
Theory-Led Design of Chiral Catalysts

12:25 – 13:00 Rong-Zhen Liao
Challenges in Modeling Water Oxidation Reactions

13:00 – 14:30 Lunch

14:30 – 15:05 Fahmi Himo
Quantum Chemical Modeling of Reactions in Confined Spaces

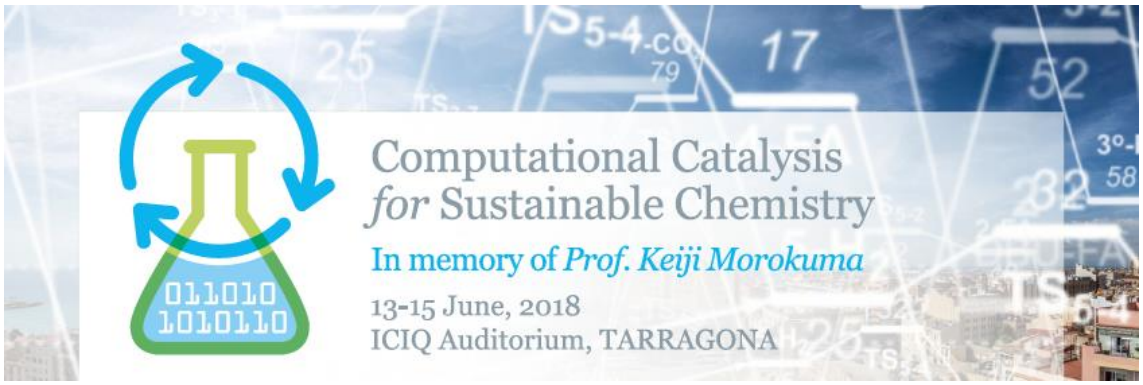
15:05 – 15:40 Maytal Toroker
Proton transfer through the bulk and near surface catalysis in nickel oxides

15:40 – 16:15 Ataualpa Braga
Computational studies on ligand-free Heck reactions

16:15 – 16:50 ioChem-BD team
The ioChem-BD platform: a Big Data solution for computational chemistry

16:50 – 19:00 Poster Session

21:00 Symposium Dinner



Friday, 15th June

9:00 – 9:35 Franziska Schoenebeck
Selective Catalysis – Insight and Application

9:35 – 10:10 Steven Wheeler
Automated Computational Workflows for Asymmetric Catalyst Design

10:10 – 10:45 Natalie Fey
Data-Driven Catalyst Discovery and Optimisation

10:45 – 11:15 Coffee Break

11:15 – 11:50 Per-Ola Norrby
Virtual Screening in Asymmetric Catalysis

11:50 – 12:25 Ainara Nova
New Approaches to the Conversion of CO2 to Methanol and Polycarbamates

12:25 – 13:00 Jeremy Harvey
Mechanism and Kinetics in Homogeneous Catalysis: A Computational Viewpoint

13:15 – 13:30 Closing Ceremony