Catalysis Sciences & Engineering [CE]
Morning Session – B6.004
Chair: Cecilia Mondelli, Sulzer & Vladimir Paunovic, ETHZ

Session Endowment: Casale SA

10:45 **Selectivity and stability of zeolite catalysts in methanol-to-hydrocarbons reaction [CE-011]**
Nikolay Kosinov, TU Eindhoven

11:15 **Consequence of Alloying and metal-oxide interface in bimetallic PtGa Propane Dehydrogenation catalysts prepared via Surface Organometallic Chemistry on Carbon [CE-013]**
Enzo Brack, ETH Zurich
M. Plodinec, C. Copéret, M. G. Willinger

11:30 **Advancing Strategies for Methane Partial Oxidation to a Methyl Ester with Heterogeneous Catalysts [CE-014]**
Andrea Blankenship, ETH Zurich
Y. Ji, M. Ravi, M. A. Newton, J. A. van Bokhoven

11:45 **Sustainable Bio-Based Solvents with Acetal Functionalized Carbohydrate Core Produced from Renewable Biomass [CE-015]**
Anastasiia Komarova, EPFL Lausanne
J. Luterbacher

12:00 **Digitally-guided synthesis of single-atom heterogeneous catalysts by leveraging language models and protocol standardization [CE-016]**
Manu Suvarna, ETH Zurich
A. Vaucher, S. Mitchell, T. Laino, J. Pérez-Ramírez

12:15 **Green Chemicals: The Ultimate Win-Win Solution Amidst Europe's Energy Crisis [CE-017]**
Abhinandan Nabera, ETH Zurich
I. R. Istrate, A. J. Martín, J. Pérez-Ramírez, G. Guillén Gosálbez

Afternoon Session – B6.004
Chair: Martin Albrecht, University of Bern

14:30 **How to overcome challenges in Green Ammonia through a multisciplinary research in catalysis [CE-021]**
Pierdomenico Biasi, Casale SA
C. Pizzolitto, R. Ostuni

15:00 **Understanding enzyme-nanoparticle interactions during bioelectrocatalytic hydrogen formation [CE-023]**
Sophie Webb, University of Geneva

15:15 **Biocatalytic reduction of six-membered ring heterocyclic imines in continuous flow [CE-024]**
Ana Benítez-Mateos, University of Bern
D. Roura Padrosa, D. Lim, V. Marchini, H. Wu, F. Buono, F. Paradisi

15:30 **CO_2 Hydrogenation to Methyl Formate using CO_2 as the Sole Carbon Source [CE-025]**
Roland Turnell-Ritson, EPFL Lausanne
P. J. Dyson

15:45 **Selective olefin transfer hydrogenation of unsaturated carbonyls with ethanol using a PYA ruthenium(II) complex [CE-026]**
Alicia Beaufils, University of Bern
M. Albrecht

16:00 **Mixed-metal Ionothermal Synthesis of Metallophthalocyanine Covalent Organic Frameworks for CO_2 Capture and Conversion [CE-027]**
Kyung Seob Song, University of Fribourg
P. W. Fritz, D. F. Abbott, L. N. Poon, C. M. Caridade, V. Mougel, A. Coskun

Computational Chemistry [CC]
Morning Session – B6.102
Chair: Jeremy Richardson, ETH Zurich

Session Endowment: Arcondis

10:45 **Invited talk Computational Chemistry [CC-011]**
Speaker tbd.

11:15 **Capturing tunnelling, wavepacket splitting and single vibronic level excitation effects on vibronic spectra with Hagedorn wavepackets [CC-013]**
Zhan Tong Zhang, EPFL Lausanne
J. Vaníček

11:30 **A local diabatisation method for two-state adiabatic conical intersections [CC-014]**
Eva Vandaele, University of Zurich
M. Mališ, S. Luber

11:45 **A DMRG-based Framework for Large-scale Quantum Many-body Calculations [CC-015]**
Nina Glaser, ETH Zurich
A. Baiardi, M. Reiher

12:00 **Heavy-atom tunneling in singlet oxygen deactivation in water [CC-016]**
Imaad Ansari, ETH Zurich
E. R. Heller, G. Trenins, J. O. Richardson

12:15 **Solvation Free Energies of Ion Dissociations in Dichloromethane: En Route to Accurate Computations [CC-017]**
Adélaïde Savoy, ETH Zurich
E. Paenurk, R. Pollice, P. H. Hünenberger, P. Chen

Afternoon Session – B6.102
Chair: Jeremy Richardson, ETH Zurich

14:30 **Computational chemistry in the life sciences industries [CC-021]**
Anna Feldman-Salit, Arcondis Group, Allschwil

15:00 **Grand canonical ensemble approaches for modeling electrochemical problems at constant electrode potentials in CP2K [CC-023]**
Ziwei Chai, University of Zurich
S. Luber

15:15 **Transition Metal Binding Site Predictions for Drug Design Applications [CC-024]**
Andrea Levy, EPFL Lausanne
S. L. Dürr, U. Röthlisberger

15:30 **Augmented Memory: Capitalizing on Experience Replay to Accelerate De Novo Molecular Design [CC-025]**
Jeff Guo, EPFL Lausanne
P. Schwaller

15:45 **Disconnection-Aware Triple Transformer Loop with a Route-Penalty Score for Multistep Retrosynthesis [CC-026]**
David Kreutter, University of Bern
J. L. Reymond

16:00 **Geometric Constraints in Probabilistic Manifolds: A Bridge from Molecular Dynamics to Structured Diffusion Processes [CC-027]**
Justin Diamond, University of Basel
M. A. Lill