

Catalysis Sciences & Engineering [CE]
Morning Session – PER 21, C140
 Chair: Vladimir Paunovic, ETH Zurich



Session Endowment: Carbogen Amcis

- 10:45 **Minimalistic Models of Oxotransferases as Catalysts for Site and Enantioselective Oxidation of Strong C-H Bonds [CE-011]**
 Miquel Costas, Universitat de Girona
- 11:15 **Developemnt of a self-optimizing platform for flow-based peptide synthesis [CE-013]**
 Bálint Tamás, University of Zurich
 P. L. Willi, H. Bürgisser, N. Hartrampf*
- 11:30 **Tracking Active Site Formation in Cu-Exchanged Zeolites for Partial CH₄ Oxidation [CE-014]**
 Andreas Brenig, ETH Zurich/PSI
 J. W. Fischer, D. Klose, G. Jeschke, J. A. van Bokhoven*, V. L. Sushkevich*
- 11:45 **CO₂ electroreduction to long-chain hydrocarbons on cobalt catalysts [CE-015]**
 Phil Preikschas, ETH Zurich
 J. Zhang, R. R. Seemakurthi, Z. Lian, A. J. Martín, S. Xi, N. López, B. Yeo, J. Pérez-Ramírez*
- 12:00 **Decoding the Promotional Effect of Iron in Bimetallic Pt-Fe-Nanoparticles for the Low Temperature Reverse Water-Gas Shift Reaction [CE-016]**
 Colin Hansen, ETH Zurich; W. Zhou, C. Copéret*
- 12:15 **Accelerating transfer hydrogenation of sterically hindered ketones with a novel mono-substituted amino-carbene (MAC) ruthenium complex [CE-017]**
 Giacomo Rigoni, University of Bern
 M. Casciotti, T. Belderrain, P. Pérez*, M. Albrecht*

Afternoon Session – PER 21, C140
 Chair: Cecilia Mondelli, Sulzer

- 14:30 **First Industrial (Total) Synthesis of Amanitin Derivatives [CE-021]**
 Emad El Sayed, Carbogen Amcis AG
 A. Krotz, K. Williams, L. Shapely, P. Brown, J. Bowen, I. Sulaiman, E. Lauterbach, J. Kovacs, S. Ruppenthal, B. Vivant, L. Mannocci, M. Doll, A. Osypenko, W. Simon, C. Lutz, C. Müller
- 15:00 **Operando XAS-XRD Reveals Structural Dynamics in CoPt Nanoparticles under Dry Reforming of Methane Conditions [CE-023]**
 David Niedbalka, ETH Zurich
 M. Janak, D. Piankova, N. Zimmerli, P. M. Abdala, C. R. Müller*
- 15:15 **Engineering a Dual-Functionalized PolyHIPE Resin for Photobiocatalytic Flow Chemistry [CE-024]**
 Emmanouil Broumidis, University of Bern
 F. Paradisi*
- 15:30 **Ruthenium-NHC complexes as precursors for highly active lignin hydrogenolysis catalysts [CE-025]**
 Lindsey Frederiksen, EPFL Lausanne
 P. Dyson*
- 15:45 **Multi-origin and topology-dependent selectivity in the methanol-to-olefins process from transient operando DRIFTS-GC [CE-026]**
 Luca Maggiulli, PSI
 J. A. Van Bokhoven, D. Ferri*
- 16:00 **Design and Characterisation of a de novo Gold Artificial Metalloenzyme [CE-027]**
 Elinor Morris, University of Basel
 J. Uhrhan, B. Lozhkin, S. Basler, I. Kalvet, T. R. Ward*, D. Baker*

Computational Chemistry [CC]
Morning Session – PER 21, C120
 Chair: Sandra Luber, University of Zurich



Session Endowment: Johnson&Johnson Innovative Medicine

- 10:45 **Simulating non-adiabatic dynamics in molecules: methodological aspects and attochemical applications [CC-011]**
 Morgane Vacher, Nantes Université
- 11:15 **From capture to catalysis: Insights from atomistic simulations into MOF and COF host-guest interactions and guest dynamics [CC-013]**
 Michelle Ernst, University of Zurich
 J. Hutter*
- 11:30 **Unravelling Tunnelling Effects in Photosensitization using Instanton Theory [CC-014]**
 Meghna Manae, ETH Zurich
 J. Richardson*
- 11:45 **Ab initio simulation of single vibronic level fluorescence spectra using Hagedorn wavepacket [CC-015]**
 Zhan Tong Zhang, EPFL Lausanne
 J. Vanicek*
- 12:00 **Accelerating Alchemical Free-Energy Calculation with the RE-EDS Multistate Method [CC-016]**
 Candide Champion, ETH Zurich
 R. Gall, B. Ries, S. Rieder, E. Pécora de Barros, P. Hünenberger*, S. Riniker*
- 12:15 **Automated Chemical Reaction Network Exploration of Oxidative Water Treatment [CC-017]**
 Enric Petrus, Eawag, Dübendorf
 U. von Gunten, M. Reiher, T. B. Hofstetter*

Afternoon Session – PER 21, C120
 Chair: Kjell Jorner, ETH Zurich

- 14:30 **Computational approaches in pharma on chemical reactivity and affinity optimization [CC-021]**
 Herman Van Vlijmen, Johnson & Johnson Innovative Medicine R&D
- 15:00 **Applying a well-defined energy density for machine-learned density functionals [CC-023]**
 Elias Polak, University of Fribourg
 S. Vuckovic, H. Zhao
- 15:15 **Inverse Design of Singlet Fission Materials with Uncertainty-Controlled Genetic Optimization [CC-024]**
 Luca Schaufelberger, ETH Zurich
 R. Laplaza, J. T. Blaskovits, C. Corminboeuf*, K. Jorner*
- 15:30 **Saturn: Sample-efficient Generative Molecular Design using Memory Manipulation [CC-025]**
 Jeff Guo, EPFL Lausanne
 P. Schwaller*
- 15:45 **A Metadynamics Study of Water Oxidation Reactions at (001)-WO₃/liquid-water Interface [CC-026]**
 Rangsiman Ketkaew, University of Zurich
 F. Creazzo, K. Sivula, S. Luber*
- 16:00 **Global and Local Electrophilicity as Measure of Endocrine Disruptor Genotoxicity Potential [CC-027]**
 Sophia Johnson, EPFL Lausanne
 S. Guilbert, U. Rothlisberger*