Program

Keynotes

KN01 – Pr. Sophia HAUSSENER, EPFL, Switzerland
Modeling and Optimization of Multi-Component and Mesostructured Photoelectrodes and Photoelectrochemical Devices
KN02 – Pr. Anastassia ALEXANDROVA, UCLA, USA
Supported Cluster Catalysts Set in Motion by Reaction Conditions: How to Model, Understand, and Tame this Dynamics
KN03 – Pr. Zhi-Pan LIU, Fudan University, Shanghai, China
Exploring Catalytic Reactions with Global Neural Network Based Methods
KN04 – Pr. Luigi CAVALLO, KAUST, Saoudi Arabia
Predicting improved catalysts using machine-learning with extra small datasets
KN05 – Pr. Inaki TUNON, University of Valencia, Spain
Efficient Simulations of Complex Catalytic Processes. Reactivity and Inhibition of the SARS-CoV-2 3CL Protease
KN06 – Pr. Evgeny PIDKO, TU Delft, The Netherlands
Bias-free operando modelling approaches to unravel the nature of extra-framework catalytic ensembles in zeolites
KN7 – Pr. Yousung JUNG, KAIST, South Korea
Data-driven multiscale models to understand and design electrocatalysts
KN8 – Pr. Emilie GAUDRY
Intermetallic compounds: (nano)-structured surfaces and electronically modified active sites for efficient catalysis
KN09 – Pr. Beatriz ROLDAN CUENYA, FHI, Berlin, Germany
Nanocatalysts in Energy Conversion
KN10 – Pr. Anatoly I. FRENKEL, Stony Brook University, NY, USA
Decoding Reactive Structures in Catalysts by Machine Learning Analysis
KN11 – Pr. Francesca BALETTO, King's College London, UK
Born different: modelling the formation of nanoparticles and nanoalloys and their consequences on catalysis
KN12 – Pr. Fabio BUSNENGO, Instituto de Fisica Rosario, Argentina
Expected, unexpected and controversial role of "defects" on chemisorption of methane on transition metal surfaces
KN13 – Pr. Tomas BUCKO, Comenius University, Slovakia
Ab initio free energy calculations at multiple electronic structure levels made affordable: An effective combination of perturbation theory and machine learning

Communications

C01 – Dorota RUTKOWSKA-ZBIK
DFT mechanistic studies on light-assisted methane coupling over Au_n/TiO_2 system

C02 – Robert JONES
Multiscale screening of plasmon enhanced photocatalysts

C03 – Vaidish SUMARIA
Modelling CO-induced Pt reconstruction using DFT-trained Neural Network Potential

C04 – Elisa JIMENEZ-IZAL
Making Pt highly CO-tolerant and highly active for Hydrogen Oxidation

C05 – Giovanni DI LIBERTO
Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts

C06 – Dmitry SHARAPA
Three stories of Copper in Catalysis

C07 – Ali HASHEMI
GARNA: Graph-based automated reaction network analysis for computational homogeneous catalysis

C08 – Paul FLEURAT-LESSARD
Theoretical investigation of cooperativity in gold catalysis

C09 – Matthew QUESNE
Reengineering the active site of non-heme iron enzymes using an expanded genetic code

C10 – Adrien HELLIER
Stability and coordination shell of Pt single atoms supported on alumina during calcination and reduction

C11 – Massimo BOCUS
Towards a realistic modelling of complex zeolite-catalysed reactions: the case of guaiacol demethylation

C12 – Fabian BERGER
The Influence of the Active Site Location in the Zeolite H-MFI on Cracking of Linear Alkanes

SCM – Fedor GOUMANS
EU collaboration opportunities to improve multi-scale modelling for catalysis

C13 – Saber GUEDDIDA
Catalytic upgrading of biomass using metallic clusters supported on amorphous silica surfaces

C14 – Laura LAVERDURE
A DFT investigation into the pH-dependency of glycerol electro-oxidation on gold

C15 – Hristiyan ALEKSANDROV
DFT modelling of the interaction of NO and NO_2 with ceria-based systems

C16 – Agustin SALCEDO
Coexisting phases of Pd-ceria catalysts for methane oxidation explored by a joint theoretical and experimental vibrational study

C17 – Igor KOWALEC
Cu, Pd and Zn surfaces for CO_2 activation and hydrogenation
C18 – Nestor Aguirre
Automated Exploration of Energy Landscapes: A Key Tool for Multiscale Materials Modeling
C19 - Nina Michelle SACKERS
Mechanistic Insights into the Ru-Catalysed Hydrogenolysis of Methanol
C20 – Michail STAMATAKIS
Single-atom alloys and highly dilute alloys as catalysts for emissions control
C21 – Etienne HESSOU
Competitive adsorption of ruthenium tetroxide vis-a-vis of water vapor, HNO_3 and NO_x on the RuO_2 surface
C22 – Pau FERRI VICEDO
Theoretical study of alkene diffusion through different small-pore zeolites
C23 – Jorge j. CARBÃ
Developing reactive force fields for propene on Pt surfaces and supported clusters
C24 – Pierre-Adrien PAYARD
Metadynamics Exploration of Supported Nanoparticles
C25 – Sanjana SRINIVAS - Spin crossing kinetics by atomically dispersed Co(II) species on an am-SiO2 substrate
C26 – Romain REOCREUX
Alkane activation on RhCu single-atom alloy: first-principles design and kinetics.
C27 – Tobias BINNINGER
The Ir-OOOO-Ir Transition State and the "Classical" Mechanism of the Oxygen Evolution Reaction on IrO_2 (110)
C28 – Simran KUMARI
Computational elucidation of active sites for electrochemical Oxygen Evolution Reaction on ITO supported Pt-ingle atom.
C29 – Monika GESVANDTNEROVA
Investigation of monomolecular isobutanol to butenes transformations catalysed by acidic zeolites
C30 – Arno DE REVIERE
Mechanistic investigation of n-butanol/ethanol dehydration in HZSM-5