

Session Program

7-11 May 2023



Operando VII

Contributed presentations

Grindelwald, Sunstar Hotel
Dorfstrasse 168, 3818 Grindelwald Switzerland

Sunday 7 May

14:30	Contributed presentations: Operando XAS at high pressure: the case of direct synthesis of hydrogen peroxide Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Dmitry Doronkin
14:50	Contributed presentations: The NO-N₂O-SCR reaction: a catalytic and spectroscopic investigation Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Filippo Buttignol
15:10	Contributed presentations: Identifying the active sites and their kinetics for butadiene synthesis from ethanol for ZnO/SiO₂, ZrO₂/SiO₂, and ZnO-ZrO₂/SiO₂ Catalysts by modulation excitation infrared spectroscopy Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Israel Wachs
16:00	Contributed presentations: Chasing adorbates and metal particle state for ceria supported Rh and Pt during CO₂ methanation and CO oxidation conditions Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Per-Anders Carlsson
16:20	Contributed presentations: Genesis of active Pt/CeO₂ catalyst for dry reforming of methane by reduction and aggregation of isolated Platinum atoms into clusters Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Simon Bare
16:40	Contributed presentations: Operando FTIR study of the understanding reactional mechanisms of the decomposition of N₂O under real industrial conditions Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Mathias Laluc
17:00	Contributed presentations: Mechanistic studies of continuous glucose upgrading over Lewis acidic silicates by operando UV-Vis and HSQC NMR Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Ceri Hammond
17:20	

Monday 8 May

10:00	Contributed presentations: Operando characterization of Fischer-Tropsch synthesis products in a fixed-bed reactor by magnetic resonance Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Qingyuan Zheng
10:20	Contributed presentations: Oxidation of Hägg carbide during high temperature Fischer-Tropsch synthesis: Size-dependent thermodynamics and in-situ observations Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Michael Claeys
10:40	Contributed presentations: Operando XAS-tomography reveals chemical gradients in Pt/Al₂O₃ and Cu-SSZ-13 emissions control catalysts Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Srashtasrita Das
11:10	Contributed presentations: Spatiotemporal operando methodologies on the reactor scale for mechanistic and kinetic studies Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Atsushi Urakawa
11:30	Contributed presentations: Insights on Rh and Pt nanoparticle dynamics by operando XAS spectroscopy during CO₂ activation via reverse water gas shift Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Chiara Negri
11:50	Contributed presentations: Dynamic evolution of Pd single atoms on anatase TiO₂ under RWGS reaction conditions Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Janos Szanyi
12:10	Contributed presentations: Mechanistic insights into reverse water gas shift reaction over Au supported catalysts by operando spectroscopic techniques Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Abdallah ahmed
14:00	Contributed presentations: Assessing the structure of SiO₂-supported Ni-Ga nanoparticles under CO₂ hydrogenation to methanol conditions via in-situ X-ray absorption, total scattering and infrared experiments Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Nora Zimmerli
14:20	Contributed presentations: A UV-Vis/ATR-IR operando spectroscopy approach to study photo-active metal-organic frameworks Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Bettina Baumgartner
14:40	
15:00	
15:20	

15:20

Contributed presentations: In situ monitoring by X-ray absorption spectroscopy of the synthesis and catalytic behavior of carbon-supported Pt single-atom catalysts in acetylene hydrochlorination

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Vera Giulimondi

15:40

16:40

Contributed presentations: Understanding the structural evolution of the most active PdZn nanoparticles used for CO₂ activation

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Sofia Mediavilla Madrigal

17:00

17:00

Contributed presentations: Quantitative transient IR analyses of CO₂ hydrogenation to methanol over Cu/ZrO₂ reveal Cu-bound formates as main reaction intermediates

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Frédéric Meunier

17:20

17:20

Contributed presentations: Catalysis operando studies combined with computed X-ray diffraction tomography: Coke formation during conversion of Methanol to Gasoline

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Lars Lundsgaard

17:40

Tuesday 9 May

09:30

Contributed presentations: Operando experiments and DFT calculations to understand the chemistry of electrocatalytic oxygen evolution

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Detre Teschner

09:50

Contributed presentations: Characterizing small metallic nanoparticles with operando X-ray scattering techniques during electrocatalysis

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Rebecca Pittkowski

10:10

Contributed presentations: Understanding the cycling performance of LiMn₂O₄ spinel nanoparticles achieved by operando XAS spectroscopy

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Juliana Bruneli Falqueto

10:30

Contributed presentations: Modulated excitation operando FT-IR and quick-X-ray absorption spectroscopy of electrooxidation over Ni-based catalysts

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Charlotte Vogt

11:20

Contributed presentations: Reaction-induced restructuring in dilute alloy catalysts

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Anatoly Frenkel

11:40

Contributed presentations: Transient APXPS as a tool to characterize the kinetics of alloy restructuring: application to Sn-poor PtSn ALD-derived nanoparticles

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Evgeniy Redekop

12:00

Wednesday 10 May

10:00	Contributed presentations: Self-sustained oscillatory dynamics of ethylene to syngas by operando SEM and XPS
10:20	Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Claudiu Colbea
10:20	Contributed presentations: 3D strain dynamics during CO oxidation revealed by Bragg-CDI
10:40	Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Amélie Rochet
11:10	Contributed presentations: Spatiotemporal operando UV-Vis spectroscopy on the reactor scale
11:30	Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Louise van Beek
11:30	Contributed presentations: Site-dependent analysis of sulfur poisoning impact on H₂ dissociation and sorption on Pd nanoparticles with operando IR nano-spectroscopy
11:50	Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Elad Gross
11:50	Contributed presentations: Operando spectroscopies and olefin polymerization catalysis: a rare marriage with a lot of unexplored potentials
12:10	Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Elena Groppo
14:00	Contributed presentations: Catalysts for dehydroaromatization of methane: insights from operando spectroscopy
14:20	Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Nikolay Kosinov
14:20	Contributed presentations: EPR investigation of metal oxide catalysts: carbon dioxide to methanol conversion induced by oxygen vacancies
14:40	Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Mikhail Agrachev
14:40	Contributed presentations: Tuning metal-support interactions in the CO₂ hydrogenation over Ni/TiO₂
15:00	Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Angela Melcherts
15:00	Contributed presentations: Cu-MOFs as oxygenation catalysts: an operando XAS study
15:20	Session Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland Convener: Matteo Signorile

15:20

Contributed presentations: Unravelling metal ratio-dependent synergistic effects in bimetallic CO₂ hydrogenation catalysts by operando X-ray absorption and infrared spectroscopy

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Dr Nina Genz

15:40

Contributed presentations: Operando DRIFT study of highly disperse CeO₂ nanoparticles supported on MgO hexagonal plates during toluene oxidation

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Alejo Aguirre

17:00

Contributed presentations: Attenuation of dimethyl ether formation from the reaction of methanol over an alumina-based methyl chloride synthesis catalyst

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** David Lennon

17:20

Contributed presentations: Localised thermal levering events drive spontaneous kinetic oscillations in catalysis

Session | Location: Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Peter Wells

17:40