

## **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

14:50

### **Contributed presentations: The NO-N<sub>2</sub>O-SCR reaction: a catalytic and spectroscopic investigation**

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Filippo Buttignol

15:10

15:40

### **Contributed presentations: Identifying the active sites and their kinetics for butadiene synthesis from ethanol for ZnO/SiO<sub>2</sub>, ZrO<sub>2</sub>/SiO<sub>2</sub>, and ZnO-ZrO<sub>2</sub>/SiO<sub>2</sub> Catalysts by modulation excitation infrared spectroscopy**

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Israel Wachs

16:00

16:00

### **Contributed presentations: Chasing adorbates and metal particle state for ceria supported Rh and Pt during CO<sub>2</sub> methanation and CO oxidation conditions**

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Per-Anders Carlsson

16:20

16:20

### **Contributed presentations: Genesis of active Pt/CeO<sub>2</sub> 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

16:40

### **Contributed presentations: Operando FTIR study of the understanding reactional mechanisms of the decomposition of N<sub>2</sub>O under real industrial conditions**

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Mathias Laluc

17:00

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

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

11:10

### **Contributed presentations: Operando XAS-tomography reveals chemical gradients in Pt/Al<sub>2</sub>O<sub>3</sub> and Cu-SSZ-13 emissions control catalysts**

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Srashtasrita Das

11:30

11:30

### **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

11:50

11:50

### **Contributed presentations: Insights on Rh and Pt nanoparticle dynamics by operando XAS spectroscopy during CO<sub>2</sub> activation via reverse water gas shift**

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Chiara Negri

12:10

14:00

### **Contributed presentations: Dynamic evolution of Pd single atoms on anatase TiO<sub>2</sub> under RWGS reaction conditions**

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Janos Szanyi

14:20

14:20

### **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

14:40

14:40

### **Contributed presentations: Assessing the structure of SiO<sub>2</sub>-supported Ni-Ga nanoparticles under CO<sub>2</sub> 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

15:00

15:00

### **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

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 CO<sub>2</sub> 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 CO<sub>2</sub> hydrogenation to methanol over Cu/ZrO<sub>2</sub> 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 Lundegaard

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

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

10:10

### **Contributed presentations: Understanding the cycling performance of LiMn<sub>2</sub>O<sub>4</sub> spinel nanoparticles achieved by operando XAS spectroscopy**

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

10:30

11:00

### **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

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

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

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Claudiu Colbea

10:20

10:20

### Contributed presentations: 3D strain dynamics during CO oxidation revealed by Bragg-CDI

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Amélie Rochet

10:40

11:10

### Contributed presentations: Spatiotemporal operando UV-Vis spectroscopy on the reactor scale

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Louise van Beek

11:30

11:30

### Contributed presentations: Site-dependent analysis of sulfur poisoning impact on H<sub>2</sub> dissociation and sorption on Pd nanoparticles with operando IR nano-spectroscopy

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Elad Gross

11:50

11:50

### Contributed presentations: Operando spectroscopies and olefin polymerization catalysis: a rare marriage with a lot of unexplored potentials

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Elena Groppo

12:10

14:00

### Contributed presentations: Catalysts for dehydroaromatization of methane: insights from operando spectroscopy

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Nikolay Kosinov

14:20

14:20

### Contributed presentations: EPR investigation of metal oxide catalysts: carbon dioxide to methanol conversion induced by oxygen vacancies

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Mikhail Agrachev

14:40

14:40

### Contributed presentations: Tuning metal-support interactions in the CO<sub>2</sub> hydrogenation over Ni/TiO<sub>2</sub>

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Angela Melcherts

15:00

15:00

### Contributed presentations: Cu-MOFs as oxygenation catalysts: an operando XAS study

**Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Matteo Signorile

15:20

15:20

**Contributed presentations: Unravelling metal ratio-dependent synergistic effects in bimetallic CO<sub>2</sub> 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

16:40

**Contributed presentations: Operando DRIFT study of highly disperse CeO<sub>2</sub> nanoparticles supported on MgO hexagonal plates during toluene oxidation****Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Alejo Aguirre

17:00

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

17:20

**Contributed presentations: Localised thermal leveraging events drive spontaneous kinetic oscillations in catalysis****Session** | **Location:** Grindelwald, Sunstar Hotel , Dorfstrasse 168, 3818 Grindelwald Switzerland | **Convener:** Peter Wells

17:40