Program of Operando VII

Sunday, 7 May 2023

12.00 – Lunch

13.50 – Welcome

14.00 **K1 – O. Safonova**, Design of XAS experiments for uncovering active sites in heterogeneous catalysts

14.30 **O1 – D. Doronkin**, Operando XAS at high pressure: the case of direct synthesis of hydrogen peroxide

14.50 **O2 – F. Buttignol**, The NO-N_2O-SCR reaction: a catalytic and spectroscopic investigation

15.10 – Coffee break

15.40 **O3 – I. Wachs**, Identifying the active sites and their kinetics for butadiene synthesis from ethanol for ZnO/SiO_2, ZrO_2/SiO_2, and $ZnO\text{-}ZrO_2/SiO_2$ Catalysts by modulation excitation infrared spectroscopy

16.00 **O4 – P.A. Carlsson**, Chasing adorbates and metal particle state for ceria supported Rh and Pt during CO_2 methanation and CO oxidation conditions

16.20 **O5 – S. Bare**, Genesis of active Pt/CeO_2 catalyst for dry reforming of methane by reduction and aggregation of isolated Platinum atoms into clusters

16.40 **O6 – M. Laluc**, Operando FTIR study of the understanding reactional mechanisms of the decomposition of N_2O under real industrial conditions

17.00 **O7 – C. Hammond**, Mechanistic studies of continuous glucose upgrading over Lewis acidic silicates by operando UV−Vis and HSQC NMR

18.50 – Opening ceremony

19.00 **P1 – F. Renz**, In situ Mössbauer spectroscopy on Mars

20.00 – Welcome dinner

Monday, 8 May 2023

9.00 **P2 – J.D. Grunwaldt**, Materials for clean air, selective oxidation and sustainable chemicals: Probing catalysts at various complexity scales by operando spectroscopy and microscopy

10.00 **O8 – Q. Zheng**, Operando characterization of Fischer-Tropsch synthesis products in a fixed-bed reactor by magnetic resonance

10.20 **O9 – M. Claeys**, Oxidation of Hägg carbide during high temperature Fischer-Tropsch synthesis: Size-dependent thermodynamics and in-situ observations

10.40 – Coffee break

11.10 **O10 – S. Das**, Operando XAS-tomography reveals chemical gradients in Pt/Al_2O_3 and Cu-SSZ-13 emissions control catalysts

11.30 **O11 – A. Urakawa**, Spatiotemporal operando methodologies on the reactor scale for mechanistic and kinetic studies

11.50 **O12 – C. Negri**, Insights on Rh and Pt nanoparticle dynamics by operando XAS spectroscopy during CO_2 activation via reverse water gas shift

12.20 Lunch

13.30 **K2 – T. Toyao**, In situ and operando spectroscopic study for multi-elemental reverse water-gas shift catalysts identified using extrapolative machine learning approach

14.00 **O13 – J. Szanyi**, Dynamic evolution of Pd single atoms on anatase TiO_2 under RWGS reaction conditions

14.20 **O14 – A. Ahmed**, Mechanistic insights into reverse water gas shift reaction over Au supported catalysts by operando spectroscopic techniques

14.40 **O15 – N. Zimmerli**, Assessing the structure of SiO_2-supported Ni-Ga nanoparticles under CO_2 hydrogenation to methanol conditions via in-situ X-ray absorption, total scattering and infrared experiments

15.00 **O16 – B. Baumgartner**, A UV-Vis/ATR-IR operando spectroscopy approach to study photo-active metal-organic frameworks

15.20 **O17 – V. Giulimondi**, In situ monitoring by X-ray absorption spectroscopy of the synthesis and catalytic behavior of carbon-supported Pt single-atom catalysts in acetylene hydrochlorination

15.40 – Coffee break

16.10 **K3 – M. Monai**, Restructuring of titanium oxide overlayers over nickel nanoparticles during catalysis as probed with operando electron microscopy and infrared spectroscopy

16.40 **O18 – S. Mediavilla Madrigal**, Understanding the structural evolution of the most active PdZn nanoparticles used for CO_2 activation

17.00 **O19 – F. Meunier**, Quantitative transient IR analyses of CO_2 hydrogenation to methanol over Cu/ZrO_2 reveal Cu-bound formates as main reaction intermediates

17.20 **O20 – L.F. Lundegaard**, Catalysis operando studies combined with computed X-ray diffraction tomography: Coke formation during conversion of Methanol to Gasoline

17.40 – Poster session

19.30 – Swiss evening

Tuesday, 9 May 2023

9.00 **K4 – E. Fabbri**, Steps towards understanding the oxygen evolution reaction enigma by operando quick X-ray absorption spectroscopy

9.30 **O21 – D. Teschner**, Operando experiments and DFT calculations to understand the chemistry of electrocatalytic oxygen evolution

9.50 **O22 – R. Pittkowski**, Characterizing small metallic nanoparticles with operando X-ray scattering techniques during electrocatalysis

10.10 **O23 – J. Bruneli Falqueto**, Understanding the cycling performance of LiMn2O4 spinel nanoparticles achieved by operando XAS spectroscopy

10.30 – Coffee break

11.00 **O24 – C. Vogt**, Modulated excitation operando FT-IR and quick-X-ray absorption spectroscopy of electrooxidation over Ni-based catalysts

11.20 **O25 – A. Frenkel**, Reaction-induced restructuring in dilute alloy catalysts

11.40 **O26 – E. Redekop**, Transient APXPS as a tool to characterize the kinetics of alloy restructuring: application to Sn-poor PtSn ALD-derived nanoparticles

12.00 **O27 – H.A. Suarez Orduz**, In situ/operando spectroscopy of emission control catalysts with tender X-rays

12.20 – Lunch

Free program

18.00 – Poster session

19.00 – Dinner

20.00 – Discussion panels: **Operando at synchrotron facilities: Quo Vadis?**

Operando cell design

Wednesday, 10 May 2023

9.00 **P3 – E. Stach**, Operando, multimodal characterization of bimetallic catalysts with electrons and x-rays

10.00 **O28 – C. Colbea**, Self-sustained oscillatory dynamics of ethylene to syngas by operando SEM and XPS

10.20 **O29 – A. Rochet**, 3D strain dynamics during CO oxidation revealed by Bragg-CDI

10.40 – Coffee break

11.10 **O30 – L. van Beek**, Spatiotemporal operando UV-Vis spectroscopy on the reactor scale

11.30 **O31 – E. Gross**, Site-dependent analysis of sulfur poisoning impact on H_2 dissociation and sorption on Pd nanoparticles with operando IR nano-spectroscopy

11.50 **O32 – E. Groppo**, Operando spectroscopies and olefin polymerization catalysis: a rare marriage with a lot of unexplored potentials

12.10 – Lunch

13.30 **K5 – C. Hess**, Elucidating CO_2 activation over reducible oxide catalysts using operando and transient spectroscopies

14.00 **O33 – N. Kosinov**, Catalysts for dehydroaromatization of methane: insights from operando spectroscopy

14.20 **O34 – M. Agrachev**, EPR investigation of metal oxide catalysts: carbon dioxide to methanol conversion induced by oxygen vacancies

14.40 **O35 – A.E.M. Melcherts**, Tuning metal-support interactions in the CO_2 hydrogenation over Ni/TiO_2

15.00 **O36 – M. Signorile**, Cu-MOFs as oxygenation catalysts: an operando XAS study

15.20 **O37 – N. Genz**, Unravelling metal ratio-dependent synergistic effects in bimetallic CO_2 hydrogenation catalysts by operando X-ray absorption and infrared spectroscopy

15.40 – Coffee break

16.10 **K6 – V. Briois**, Second and micrometer spatial resolution for operando characterizations of heterogeneous energy-related materials by Full Field Hyperspectral Quick-EXAFS Imaging

16.40 **O38 – A. Aguirre**, Operando DRIFT study of highly disperse CeO_2 nanoparticles supported on MgO hexagonal plates during toluene oxidation

17.00 **O39 – D. Lennon**, Attenuation of dimethyl ether formation from the reaction of methanol over an alumina-based methyl chloride synthesis catalyst

17.20 **O40 – P. Wells**, Localised thermal levering events drive spontaneous kinetic oscillations in catalysis

17.40 – Closing remarks

19.00 – Congress dinner

Thursday, 11 May 2023

9.00 – Shuttle bus to the Operando School, Paul Scherrer Institut

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