

# IWOX-14

Jan 14-19, 2024

Schladming Austria

## Program

	Sunday	Monday	Tuesday	Wednesday	Thursday	Friday	
9 <sup>00</sup> -9 <sup>45</sup>	Arrival & Registration	<b>Goniakowski</b>	<b>Paganini</b>	<b>Dohnalek</b>	<b>Cheng</b>	<b>Franceschi</b>	
9 <sup>45</sup> -10 <sup>15</sup>		<b>Surnev</b>	<b>Blanco Garcia</b>	<b>Stierle</b>	<b>Selloni</b>	<b>Custance</b>	
10 <sup>15</sup> -10 <sup>45</sup>		<b>Noguera</b>	<b>Noei</b>	<b>HajiNaghiTehrani</b>	<b>Lykhach</b>	<b>Presel</b>	
10 <sup>45</sup> -11 <sup>00</sup>		coffee break	coffee break	coffee break	coffee break	coffee break	
11 <sup>00</sup> -11 <sup>30</sup>		<b>Barth</b>	<b>Spurio</b>	<b>Meier</b>	<b>Esch</b>	<b>Riva</b>	
11 <sup>30</sup> -12 <sup>00</sup>		<b>Flege</b>	<b>Reticcioli</b>	<b>Vonbun-F.</b>	<b>Kaiser</b>	<b>Du</b>	
12 <sup>00</sup> -12 <sup>30</sup>		<b>Libuda</b>		<b>Sun</b>	Discussions	Closing	
12 <sup>30</sup> -14 <sup>00</sup>		break	Discussions	break			
14 <sup>00</sup> -14 <sup>45</sup>		<b>Altman</b>		<b>Lustemberg</b>			
14 <sup>45</sup> -15 <sup>15</sup>		<b>Smyczek</b>		<b>Huang</b>			
15 <sup>15</sup> -15 <sup>45</sup>		<b>Förster</b>		<b>Wang</b>			
15 <sup>45</sup> -16 <sup>15</sup>		coffee break		coffee break			
16 <sup>15</sup> -16 <sup>45</sup>		<b>Diebold</b>		<b>Wöll</b>			
16 <sup>45</sup> -17 <sup>15</sup>		<b>Conti</b>		<b>Kim</b>			
17 <sup>15</sup> -17 <sup>45</sup>		<b>Kaur</b>		<b>Grönbeck</b>			IWOX Board Meeting
18 <sup>30</sup> -20 <sup>00</sup>		Dinner		Dinner	Dinner	Dinner	Conference Dinner
20 <sup>00</sup> -20 <sup>45</sup>			<b>Company Presentations and Poster Pitch</b>				
20 <sup>45</sup> -22 <sup>30</sup>			<b>Poster Session</b>				

## Monday, Jan 15

9 <sup>00</sup> -9 <sup>45</sup>	Chair: M. Sterrer <b>Jacek Goniakowski (invited)</b> <i>Application of Machine-Learning Interaction Potentials to Studies of Complex Nano-Oxides: Electrostatic and Charge Transfer Effects.</i>
9 <sup>45</sup> -10 <sup>15</sup>	<b>Svetlozar Surnev</b> <i>Atomic Insights on the Structure of 2D MoO<sub>3</sub> Layers on Pd(100).</i>
10 <sup>15</sup> -10 <sup>45</sup>	<b>Claudine Noguera</b> <i>Polarity Effects in Two-Dimensional MoO<sub>3</sub> Oxide Nanostructures.</i>
10 <sup>45</sup> -11 <sup>00</sup>	Coffee break
11 <sup>00</sup> -11 <sup>30</sup>	Chair: Z. Dohnalek <b>Clemens Barth</b> <i>The Inverse Catalyst Ceria/Cu(111) and the Water-Forming Reaction on Supported Pd.</i>
11 <sup>30</sup> -12 <sup>00</sup>	<b>J. Ingo Flege</b> <i>Significant Reducibility of Atomic Layer Deposited Ultrathin Ceria Towards H<sub>2</sub> at Room Temperature.</i>
12 <sup>00</sup> -12 <sup>30</sup>	<b>Jörg Libuda</b> <i>Atomic Layer Deposition of Transition-Metal Dichalcogenides on Functionalized Oxide Interfaces: Insights from Surface Science.</i>
12 <sup>30</sup> -14 <sup>00</sup>	break
14 <sup>00</sup> -14 <sup>45</sup>	Chair: C. Wöll <b>Eric Altman (invited)</b> <i>Two-dimensional Silicates; Growth, Structure, Properties and Applications.</i>
14 <sup>45</sup> -15 <sup>15</sup>	<b>Jan S. Smyczek</b> <i>Growth of Ultrathin CoO<sub>x</sub> Films on Pd(100) and Their Interaction with Water.</i>
15 <sup>15</sup> -15 <sup>45</sup>	<b>Stefan Förster</b> <i>A Two-dimensional Aperiodic Network Hosting Eu.</i>
15 <sup>45</sup> -16 <sup>15</sup>	Coffee break
16 <sup>15</sup> -16 <sup>45</sup>	Chair: P. Luches <b>Ulrike Diebold</b> <i>Obtaining a True SrTiO<sub>3</sub>(001)-(1×1) Surface by Cleaving.</i>
16 <sup>45</sup> -17 <sup>15</sup>	<b>Andrea Conti</b> <i>Surface Reconstructions of Al<sub>2</sub>O<sub>3</sub>(0001) Predicted with Ab-Initio-Derived Force Fields.</i>
17 <sup>15</sup> -17 <sup>45</sup>	<b>Harsharan Kaur</b> <i>Investigating Sputter Deposited Iron Oxide Thin Films on Calcium Fluoride Substrates.</i>
18 <sup>30</sup>	Dinner

Tuesday, Jan 16

- 9<sup>00</sup>-9<sup>45</sup> Chair: W. Huang  
**M. Cristina Paganini (invited)**  
*Doped and mixed transition metal oxides as visible light photoactive interfaces.*
- 9<sup>45</sup>-10<sup>15</sup> **Miguel Blanco Garcia**  
*Adsorption of SARS-CoV-2 SPIKE Amino Acids, Asparagine and Cysteine, on the Surface of Model Catalyst TiO<sub>2</sub>.*
- 10<sup>15</sup>-10<sup>45</sup> **Heshmat Noei**  
*Photocatalysis at the TiO<sub>2</sub> Surface in Real Time.*
- 10<sup>45</sup>-11<sup>00</sup> Coffee break
- 11<sup>00</sup>-11<sup>30</sup> Chair: A. Stierle  
**Eleonora Spurio**  
*Structural and Electronic Properties of Photoexcited States in Cerium Oxide.*
- 11<sup>30</sup>-12<sup>15</sup> **Michele Reticioli (invited)**  
*Characterization and Effects of Polarons on Oxide Surfaces via Machine Learning.*
- 12<sup>15</sup>-18<sup>30</sup> Discussions
- 18<sup>30</sup>-20<sup>00</sup> Dinner
- 20<sup>00</sup>-20<sup>20</sup> **Marten Patt (Focus)**  
Imaging Spin Filter for NanoESCA Based on Au/Ir and Oxide Passivated Iron
- 20<sup>20</sup>-20<sup>40</sup> **Christoph D. Feldt (Specs)**  
From Fully Automated to Fully Customized – A Review of SPECS NAP-XPS System Solutions
- 20<sup>45</sup>-22<sup>30</sup> **Poster Pitch and Poster Session**

## Wednesday, Jan 17

9 <sup>00</sup> -9 <sup>45</sup>	Chair: J. Libuda <b>Zdenek Dohnalek (invited)</b> <i>Elementary Steps in Catalytic Conversion of Carboxylic Acids on Model Oxide Catalysts.</i>
9 <sup>45</sup> -10 <sup>15</sup>	<b>Andreas Stierle</b> <i>Adsorption of Carboxylic Acids on Magnetite Surfaces and Nanoparticles.</i>
10 <sup>15</sup> -10 <sup>45</sup>	<b>Mohammad Ebrahim Haji Naghi Tehrani</b> <i>Adsorption Study of Formic Acid on Magnetite NPs Supported by Al<sub>2</sub>O<sub>3</sub>(0001).</i>
10 <sup>45</sup> -11 <sup>00</sup>	Coffee break
11 <sup>00</sup> -11 <sup>30</sup>	Chair: A. Selloni <b>Matthias Meier</b> <i>Structure of Reduced Fe<sub>3</sub>O<sub>4</sub> Surfaces.</i>
11 <sup>30</sup> -12 <sup>00</sup>	<b>Gregor B. Vonbun-Feldbauer</b> <i>Atomistic Modelling of Surfaces and Interphases for Hybrid Nanocomposites.</i>
12 <sup>00</sup> -12 <sup>30</sup>	<b>Yan Sun</b> <i>Direct Observation of Active Phase of Perovskite SrIrO<sub>3</sub> for Oxygen Evolution Reaction.</i>
12 <sup>30</sup> -14 <sup>00</sup>	break
14 <sup>00</sup> -14 <sup>45</sup>	Chair: M. C. Paganini <b>Pablo Lustemberg (invited)</b> <i>Optimizing Methane Conversion to Methanol: The Role of Metal-Support Interaction and Liquid Phase in Ceria-Based Catalysis.</i>
14 <sup>45</sup> -15 <sup>15</sup>	<b>Weixin Huang</b> <i>Elementary Surface Reaction Kinetics on Working Oxide Catalysts for CO<sub>x</sub> Hydrogenation Reactions.</i>
15 <sup>15</sup> -15 <sup>45</sup>	<b>Yuemin Wang</b> <i>Structure and Chemical Reactivity of Pristine and Pt-Deposited Oxide Surfaces: An Infrared Spectroscopic Investigation.</i>
15 <sup>45</sup> -16 <sup>15</sup>	Coffee break
16 <sup>15</sup> -16 <sup>45</sup>	Chair: F. Netzer <b>Christof Wöll</b> <i>Bridging the Pressure and Materials Gap in Heterogeneous Catalysis – A Combined UHV, In Situ and Operando Study Using Infrared Spectroscopy.</i>
16 <sup>45</sup> -17 <sup>15</sup>	<b>Kyungmin Kim</b> <i>Atomic-Scale Characterization of the CeO<sub>2</sub>(100) Surface with Atomic Force Microscopy and Force Spectroscopy.</i>
17 <sup>15</sup> -17 <sup>45</sup>	<b>Henrik Grönbeck</b> <i>Oxide-Face-Dependent Structure of Pt Nanoparticles on Ceria.</i>
18 <sup>30</sup>	Dinner

## Thursday, Jan 18

9 <sup>00</sup> -9 <sup>45</sup>	Chair: U. Diebold <b>Jun Cheng (invited)</b> <i>In-situ Probing Oxide-Water Interfaces by Combining EC-STM and MLMD.</i>
9 <sup>45</sup> -10 <sup>15</sup>	<b>Annabella Selloni</b> <i>A Molecular-Scale Picture of the Electrical Double Layer at TiO<sub>2</sub>-Electrolyte Interfaces.</i>
10 <sup>15</sup> -10 <sup>45</sup>	<b>Yaroslava Lykhach</b> <i>Impact of Electronic Support Interaction on the Stability of Metal/Oxide Interfaces in Electrochemical Environment.</i>
10 <sup>45</sup> -11 <sup>00</sup>	Coffee break
11 <sup>00</sup> -11 <sup>30</sup>	Chair: Y. Du <b>Friedrich Esch</b> Does Cluster Encapsulation Inhibit Sintering? Stabilization of Size-Selected Pt Clusters on Fe <sub>3</sub> O <sub>4</sub> (001) by SMSI.
11 <sup>30</sup> -12 <sup>00</sup>	<b>Sebastian Kaiser</b> <i>Clusters vs. Nanoparticles: Encapsulation of Pt on Rutile TiO<sub>2</sub>(110).</i>
12 <sup>00</sup> -18 <sup>30</sup>	Discussions
17 <sup>00</sup> -18 <sup>00</sup>	Board meeting
18 <sup>30</sup> -20 <sup>00</sup>	Conference dinner

## Friday, Jan 19

9 <sup>00</sup> -9 <sup>45</sup>	Chair: E. Altman <b>Giada Franceschi (invited)</b> <i>How Water Adsorbs on K-Feldspars.</i>
9 <sup>45</sup> -10 <sup>15</sup>	<b>Oscar Custance</b> <i>Characterization of Molecular H<sub>2</sub>O and CO<sub>2</sub> on the CeO<sub>2</sub>(111) Surface with High-Resolution Atomic Force Microscopy.</i>
10 <sup>15</sup> -10 <sup>45</sup>	<b>F. Presel</b> <i>An STM Investigation on the CO<sub>2</sub> Activation and Conversion on Au/MgO(001) Ultrathin Film.</i>
10 <sup>45</sup> -11 <sup>00</sup>	Coffee break
11 <sup>00</sup> -11 <sup>30</sup>	Chair: M. Sterrer <b>Michele Riva</b> <i>Surfaces of La<sub>0.8</sub>Sr<sub>0.2</sub>MnO<sub>3</sub>(001) at the Atomic Scale.</i>
11 <sup>30</sup> -12 <sup>00</sup>	<b>Yingge Du</b> <i>Mg<sup>2+</sup> Diffusion Across Epitaxial Fe<sub>3</sub>O<sub>4</sub>/MgO(001) Interfaces.</i>
12 <sup>00</sup> -	Closing and departure

## Poster list

**P1 Alexander Simanenko**

*Nanoarchitected Bimetallic Pd-Rh Nanoparticles Supported on  $\text{Co}_3\text{O}_4(111)$ : Atomic Ordering and Stability.*

**P2 Ming-Chao Kao**

*Structure and Stability of Al-alloyed  $\beta\text{-Ga}_2\text{O}_3(100)$  Surfaces.*

**P3 Johanna Reich**

*Size-Selected Pt Clusters on Atomically Flat  $\text{CeO}_2/\text{Rh}(111)$  Thin Films.*

**P4 Lukas Schewe**

*XPS Study on Composition and Band Structure of Aluminum-Alloyed  $\beta$ -Gallium Oxide Bulk Crystals and Thin Films.*

**P5 Max Niederreiter**

*Interplay of Adsorption Geometry and Work Function Evolution at the TCNE/Cu(111) Interface.*

**P6 Paola Luches**

*Photoexcited States in Cerium Oxide-Based Materials Studied by Ultrafast Spectroscopies.*

**P7 Martin Sterrer**

*Manipulating the Charge State of Porphin Molecules on Ultrathin  $\text{MgO}(001)$  Films.*