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# OPERANDO SOFT X-RAY ABSORPTION SPECTROSCOPY: APPLICATION AND PERSPECTIVES

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July 4-5, 2022 | Trieste

[www.trieste.nffa.eu/xas-workshop](http://www.trieste.nffa.eu/xas-workshop)

# MONDAY | JULY 4 | MORNING

9:00-9:10 Welcome and introduction

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## SESSION 1

CHAIR: PROF. P. GHIGNA

9:10-9:40 KEYNOTE: Evaluation of the impact of the in situ cell design on the interfacial speciation over C-based electrodes during room temperature CO<sub>2</sub> electroreduction

**Rosa Arrigo**, *School of Science, Engineering and Environment, University of Salford, Manchester, UK*

9:40-10:00 X-ray 'eyes' for the description of unprecedented details in metal-organic frameworks adsorption and catalytic processes

**Valentina Colombo**, *Dipartimento di Chimica, Università degli Studi di Milano, Milan, Italy*

10:00-10:20 Insights into the Redox Behaviour of PrBaMn<sub>2</sub>O<sub>5</sub> through a multi-analysis approach

**Andrea Felli**, *Dipartimento Politecnico di Ingegneria e Architettura, Università di Udine, Udine, Italy*

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10:20-11:00 Coffee break

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## SESSION 2

CHAIR: PROF. M. STENER

11:00-11:30 KEYNOTE: Overview of the interpretation of x-ray absorption spectroscopy

**Frank De Groot**, *Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, Netherlands*

11:30-12:00 KEYNOTE: Ab initio approach to XANES: Theory and applications

**Benedikt Maurer**, *Institut für Physik and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany*

12:00-12:30 Caught while dissolving: revealing the interfacial solvation of the Mg<sup>2+</sup> ions on the MgO surface

**Paola D'Angelo**, *Dipartimento di Chimica, Sapienza Università di Roma, Rome, Italy*

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12:30-14:30 Lunch

# MONDAY | JULY 4 | AFTERNOON

## SESSION 3

CHAIR: DR. S. BENEDETTI

- 14:30-15:00** KEYNOTE: Novel low-cost materials as candidate electrocatalysts for efficient hydrogen evolution reaction: a surface-science approach  
**Antonio Politano**, *INSTM / Dipartimento di Scienze fisiche e chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy*
- 15:00-15:20** X-ray absorption spectroscopy to track local structure and reactivity of metal sites in heterogeneous catalysts  
**Elisa Borfecchia**, *Dipartimento di Chimica e Centro Interdipartimentale Superfici ed Interfasi Nanostrutturate, Università di Torino, Turin, Italy*
- 15:20-15:40** Xas spectroscopy on High Entropy Oxides: recent advances in the determination of the mechanisms of heterogeneous reactions  
**Martina Fracchia**, *Dipartimento di Chimica, Università di Pavia, Pavia, Italy*
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**15:40-16:20** Coffee break

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## SESSION 4

CHAIR: DR. S. ZAFEIRATOS

- 16:20-16:50** KEYNOTE: Disclosing the electronic properties of Ti sites in Ziegler-Natta catalysts at each step of the process  
**Alessandro Piovano**, *Dipartimento Scienza Applicata e Tecnologia, Politecnico di Torino, Turin, Italy*
- 16:50-17:10** Inverse CeO<sub>2</sub>/CuO catalyst for partial methane oxidation: a combined in situ DRIFT and operando NEXAFS study  
**Silvia Mauri**, *CNR - Istituto Officina dei Materiali, Trieste, Italy*
- 17:10-17:40** Fe(II) open metal sites in Metal-organic frameworks: spin transitions and redox properties in adsorption and catalysis  
**Marco Vandone**, *Dipartimento di Chimica, Università degli Studi di Milano, Milan, Italy*
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**19:00-20:20** Aperitif dedicated to Carlo Lamberti at the restaurant *Pier The Roof*  
Molo Venezia

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**20:30-** Social dinner at the restaurant *Il Melograno*  
Via di Cavana 14

# TUESDAY | JULY 5

## SESSION 5

CHAIR: DR. R. ARRIGO

- 9:00-9:30** KEYNOTE: Innovative workflows for correlative operando studies by electron microscopy and synchrotron spectroscopy  
*Regina Ciancio, CNR - Istituto Officina dei Materiali, Trieste, Italy*
- 9:30-9:50** Recent advances and perspectives at AP-soft XAS end-station at APE-HE  
*Piero Torelli, CNR - Istituto Officina dei Materiali, Trieste, Italy*
- 9:50-10:10** Operando soft XAS at the VerSoX beamline of Diamond Light Source  
*Georg Held, Diamond Light Source, Didcot, UK*

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**10:10-10:50** Coffee break

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## SESSION 6

CHAIR: PROF. V. COLOMBO

- 10:50-11:20** KEYNOTE: Using chemical information from operando X-ray spectroscopies to design better catalysts  
*Spiros Zafeirotos, Institut de Chimie et Procédés pour l'Énergie, l'Environnement et la Santé, CNRS - Université de Strasbourg, Strasbourg, France*
- 11:20-11:40** Soft X-Ray spectroscopy in liquids: in-situ and operando investigation at BACH beamline  
*Silvia Nappini, CNR - Istituto Officina dei Materiali, Trieste, Italy*
- 11:40-12:00** Unconventional way to apply FT-IR spectroscopy: the case of HEO characterization  
*Andrea Jouve, Dipartimento di Scienza e Tecnologia del Farmaco, Università di Torino, Turin, Italy*
- 12:00-12:20** In situ NEXAFS study to uncover defective sites in HKUST-1 MOFs  
*Luca Braglia, CNR - Istituto Officina dei Materiali, Trieste, Italy*

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**12:20-12:30** Concluding remarks