

## 15th EC<sup>2</sup>/BIG-NSE Workshop

Start Time: Thursday, December 16, 2021

End Time:



The 15th EC<sup>2</sup>/BIG-NSE Workshop will take place on Friday, January 7, 2022 as an online event. The link will be communicated a few days before start on the corresponding website of [EC<sup>2</sup>/BIG-NSE](#). As every year once their "initial phase" is finished, the [new PhD students](#) of EC<sup>2</sup>/BIG-NSE have the opportunity to present their PhD work plan in front of the UniSysCat community.

The first presentation is planned to start at about **13:10** and the last one to finish around **17:45**. The scope of the presentations ranges from theory to application on all aspects of catalysis: Organic/Inorganic chemistry, heterogeneous catalysis, biotechnologies, biocatalysis etc.: all interested scientists are welcome!

The (tentative) timetable is as follows:

**13:00-13:10** Welcome words by [Prof. Maria Andrea Mroginski](#)

**13:10-13:35** Nicole Mancini: Ab-initio prediction of adsorption isotherm of water with a metal organic framework (MOF)

**13:35-14:00** Kathrin Maria Nieswiec: Investigation of the phase transformation of a cerium-based catalyst under non-equilibrium conditions in the Deacon-process using computational methods

**14:00-14:05** Break

**14:05-14:30** Victor Nicolaus: Artificial biocatalysis with chemically or biologically synthesized molybdenum cofactors

**14:30-14:55** Cornelius Bernitzky: Exploring multifunctional hydrogenases by advanced vibrational spectroscopy: Reaction site coupling in complex biocatalytic systems

**14:55-15:20** Miriam Carmen Walczak: Structural studies on pyrimidine nucleoside phosphorylases to improve kinetics for sugar-modified nucleosides

**15:20-15:25** Break

**15:25-15:50** Shima Farhoosh: Electrochemical and light-driven water splitting tracked by operando X-ray spectroscopy

**15:50-16:15** Honghua Zuo: Silylium ion promoted electrophilic C–H silylation and cyclopropane ring opening in various ways

**16:15-16:20** Break

**16:20-16:45** Jesvita Cardozo: Carbonylation and carboxylation of alkanes in fluorinated solvents and supercritical carbon dioxide

**16:45-17:10** Wanli Ma: Tandem catalysis enabled by single-side bridging and pincer-ligated heterobimetallic complexes

**17:10-17:35** Amanda Opis Basilio: Small molecule activation regulated by secondary coordination and electrostatic effects within artificial non-heme metalloproteins

**17:35-17:40** Closing remarky by [Prof. Maria Andrea Mroginski](#)