15th EC2/BIG-NSE Workshop

Start Time: Thursday, December 16, 2021

End Time:

The 15th EC^2/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^2/BIG-NSE. As every year once their "initial phase" is finished, the new PhD students of EC^2/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